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TIME MEASUREMENT IN QUANTUM MECHANICS

by

ⓒ PAUL A. CARLSON

A THESIS

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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research, for acceptance, a thesis entitled TIME MEASUREMENT IN QUANTUM MECHANICS submitted by PAUL A. CARLSON in partial fulfillment of the requirements for the degree of Master of Science.

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ABSTRACT

A new approach is given by the author in this thesis to solve the problem of time delay and time of arrival in quantum mechanics. It is shown that time of arrival is an improper and not a proper quantum mechanical observable, since the associated operator is not self-adjoint but only Hermitian. This means that the fundamental property of self-adjoint operators, which supplies a complete orthonormal set of eigenfunctions with real eigenvalues does not apply. All the familiar results of quantum mechanics depend on this. Some authors have attempted to quantize certain functions of time of arrival in the hope of achieving self-adjointness. A different method has been selected here. Instead of attempting to construct a self-adjoint operator, the author outlined a detailed proof of all orthogonality, linearity and transformation relations directly in the case of the Hermitian time of arrival operator without reference to the general results for self-adjoint operators. In this case the time of arrival operator is linear on subspaces of the configuration Hilbert space known as time domains.

Also originated by the author, is the unique method for measuring time of arrival and hence time delay at a specified point in space, instead of time delay associated with some angular momentum quantum number ℓ. The concept of eigenfunction point phasing is introduced and is justified by examples throughout the chapters of the thesis. Time delay is discussed for one dimensional transition and simple three dimensional radially symmetric elastic scattering. As the scattering differential cross section

determines the absolute value of the scattering amplitude, time delay is shown to determine its phase. Finally, some approximation methods are discussed.

The introductory chapters prepare the way for the main theory to follow. Chapter I reviews wave mechanics and proves the uncertainty relation, and uses this result to obtain the minimum uncertainty wave packet. Chapters II and III discuss classical time delay in one dimension and three dimensions respectively. Chapter IV briefly examines the classical conjugate Hamiltonian formulation of the time function. Chapter V begins the quantum theory of time measurement.

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CHAPTER I

NON-STATIONARY STATES OF A FREE PARTICLE

A stationary state ψ for a particle in quantum mechanics is an energy eigenstate with time dependence of the form $e^{-i\omega t}$. Such a state satisfies the condition that $|\psi|^2$ is independent of time. For the one dimensional free particle equation

$$i\hbar \frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \qquad (1)$$

the stationary state solutions are $e^{i(kx-\omega t)}$ where the energy eigenvalue is $E = \hbar\omega = \frac{\hbar^2 k^2}{2m}$. The general solution to (1) which is nonstationary, can be evaluated as a linear combination of stationary states as

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} A(k)\, e^{ikx - \frac{i\hbar k^2}{2m}t}\, dk \quad . \qquad (2)$$

$A(k)$ determines the distribution of momentum components in the wavefunction ψ. The factor $\frac{1}{\sqrt{2\pi}}$ is included for Fourier transform convenience. If we define $\phi(k,t)$ by

$$\phi(k,t) = A(k)\, e^{-\frac{i\hbar k^2}{2m}t} \qquad (3)$$

then ϕ and ψ are Fourier transforms of one another, that is

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k,t)\, e^{ikx}\, dk \quad ,$$

$$\phi(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x,t)\, e^{-ikx}\, dx \quad .$$

ψ and ϕ are respectively known as the position and momentum wavefunctions. They are always related by the Fourier transform equations above, even in the case of a non-zero potential. However the time dependence of the momentum wavefunction does not have the simple form of (3) in this case. For a free particle we can write (3) as

$$\phi(k,t) = \phi(k,t_0) \exp\left[\frac{-i\hbar k^2 (t-t_0)}{2m}\right]$$

which gives the time dependence of ϕ at any future or past time in terms of the value of ϕ at t_0. Since the Fourier transform is unitary, we can express $\psi(x,t)$ in terms of the x dependence of ψ at t_0. Using (3) we can express $A(k)$ in terms of $\phi(k,t_0)$ and hence in terms of $\psi(x,t_0)$ using the inverse Fourier transform. Substituting in (2) and integrating with respect to k we obtain

$$\psi(x,t) = \frac{1-i}{2} \sqrt{\frac{m}{\pi \hbar (t-t_0)}} \int_{-\infty}^{\infty} \psi(\bar{x},t_0) \exp\left(\frac{im(x-\bar{x})^2}{2h(t-t_0)}\right) d\bar{x} \quad . \tag{4}$$

These coefficients come from the internal integration in the expression

$$\psi(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi(\bar{x},t_0) \left[\int_{-\infty}^{\infty} e^{ik(x-\bar{x}) - \frac{i\hbar k^2}{2m}(t-t_0)}\, dk\right] d\bar{x} \quad .$$

Observe that if $A(k)$ and hence $\phi(k)$ is square integrable, then so is $\psi(x,t)$ and moreover

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = \int_{-\infty}^{\infty} \psi^*(x,t)\psi(x,t) dx = \int_{-\infty}^{\infty} |\phi(k,t)|^2 dk = \int_{-\infty}^{\infty} |A(k)|^2 \, dk \, .$$

If all these integrals equal 1 , the wave packet representing the particle is said to be normalized. To show the norm preserving property of the Fourier transform which establishes the above result, we substitute the Fourier integral for ψ in terms of ϕ in the expression $\int_{-\infty}^{\infty} \psi^*\psi \, dx$ using two different integration variables k and b in the ϕ function integration. We can then separate out the delta function integral $\delta(k-b) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ix(k-b)} \, dx$. The symbol δ is not a function at all, but $\delta(k-b)$ is the kernel of an operator (the identity operator) on the linear space of Fourier transformable functions. For this we see that the Fourier transform operator F preserves norm. Thus the normalization integral is independent of time for both position and momentum wavefunctions.

Using (4) with $t_0 = 0$ if we substitute $\psi(\bar{x},0) = e^{ik\bar{x}}$ and integrate we get $\psi(x,t) = e^{ikx - i\omega t}$ which is the travelling wave which is not square integrable. On the other hand, if we take the wave packet localized at $t = t_0 = 0$, namely $\psi(\bar{x},0) = \delta(\bar{x})$ we find $\psi(x,t) = \frac{(1-i)}{2}\sqrt{\frac{m}{\pi\hbar t}} \exp\left(\frac{imx^2}{2\hbar t}\right)$ which is not normalized since $\int_{-\infty}^{\infty} |\delta(x)|^2 \, dx = \delta(0)$ which is not finite. We would have to take $\psi(\bar{x},0) = \sqrt{\delta(\bar{x})}$ to get a normalized square integrable function, but this would give $\psi(x,t) = 0$. To understand the reason for this, let us look at the case $\psi_\alpha(\bar{x},0) = \sqrt[4]{\frac{\alpha}{\pi}}\, e^{-\alpha\bar{x}^2/2}$, for $\alpha > 0$. Substituting this into the integral in (4) and evaluating (details omitted) we get

$$\psi_\alpha(x,t) = (\frac{\alpha}{\pi})^{1/4}(1 + \frac{i\hbar\alpha t}{m})^{-1/2} \exp(\frac{-\alpha x^2}{2(1 + \frac{i\hbar\alpha t}{m})}) \quad . \qquad (5)$$

From this equation (5) we can see the way a wavefunction spreads as a function of time depending on its initial configuration. If $\alpha\hbar t >> m$ we have

$$\psi_\alpha(x,t) \simeq (\frac{\alpha}{\pi})^{1/4} (\frac{i\hbar\alpha t}{m})^{-1/2} \exp(\frac{imx^2}{2\hbar t}) \quad .$$

Thus for large α , the initial configuration (which is normalized) more closely resembles $\psi_\infty(\bar{x},0) = \sqrt{\delta(\bar{x})}$ and the wavefunction $\psi_\alpha(x,t)$ approaches the form $\exp(\frac{imx^2}{2\hbar t})$ as $\alpha \to \infty$ with amplitude degenerating to zero. This explains the reason we found $\psi_\infty(x,t)$ to be zero previously.

It is apparent that the wavefunction $\psi_\alpha(x,t)$ spreads with time, and has minimum spread at time $t = 0$. For large α (initially narrow distribution) the wave packet spreads quickly, while for small positive α near zero, it spreads slowly in time. This will be shown quantitatively in the following discussion.

The expectation value of a given physical quantity A in a state ψ is represented by $\langle A\rangle_t = \int_{-\infty}^{\infty} \psi^*(x,t)\, A\, \psi(x,t)\, dx$, where ψ is normalized. Similarly, with respect to the momentum wavefunction $\langle B\rangle_t = \int_{-\infty}^{\infty} \phi^*(k,t)\, B\phi(k,t)\, dk$. A may be any operator on functions of x , and B any operator on functions of k . For the one dimensional free particle, some of the more important operators are listed below.

TABLE I

OPERATOR REPRESENTATIONS

Physical Quantity	Position Representation	Momentum Representation
Position x	x	$i \frac{\partial}{\partial k}$
Momentum / ħ = $\frac{p}{\hbar}$	$-i \frac{\partial}{\partial x}$	k
Energy = E	$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$	$\frac{\hbar^2 k^2}{2m}$
x^n	x^n	$(i \frac{\partial}{\partial k})^n$

Any of these operator equivalence can be verified. The condition for A and B to be equivalent is

$$\int_{-\infty}^{\infty} \psi^*(x)\ A\ \psi(x)\ dx = \int_{-\infty}^{\infty} \phi^*(k)\ B\ \phi(k)\ dk$$

for all functions $\phi(k)$ such that $\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\ e^{ikx}\ dk$ or $\psi = F\phi$ where F is the Fourier transform operator. This means $B = F^{-1}AF$ since F in unitary.

Now return to the function $\psi_\alpha(x,t)$. The spread of a wave-packet is equal to $\langle(x-\langle x\rangle)^2\rangle = \langle x^2\rangle - \langle x\rangle^2$. But $\langle x\rangle = 0$ for ψ_α and so $\langle(x-\langle x\rangle)^2\rangle = \langle x^2\rangle = \frac{\alpha^2\hbar^2t^2+m^2}{2m^2\ \alpha^2}$. This explicitly shows that $t = 0$ is the time of minimum spread, and that narrow distributions at $t = 0$ (large α) spread more rapidly.

For a free particle in one dimension we can demonstrate the following results, directly from the time dependence in (3) or (4), and the operators in Table I.

$<-i\hbar \frac{\partial}{\partial x}>_t = p_0 = \hbar k_0$ a constant independent of t. Moreover $k_0 = <k>_t = \int_{-\infty}^{\infty} k|A(k)|^2\, dk$, and may be positive or negative. Define $v = \frac{p_0}{m}$. Then,

$$<x>_t = v(t-t_0) + <x>_{t_0} \quad ,$$

$$E = <-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}> = <\frac{\hbar^2 k^2}{2m}> = E_d + E_t \quad \text{where} \quad E_d > 0 \quad ,$$

and $E_t = \frac{p_0^2}{2m} = \frac{1}{2} mv^2 \geq 0$. E and E_d are positive real constants independent of time. E_t is energy of translation, and the subscript does not refer to time. E_d is energy difference.

If we define $(\Delta x)^2_t = <(x-<x>_t)^2>_t$ as the spread of the wave packet, then $(\Delta x)^2_t$ is a positive quadratic in t achieving a minimum at some time t_1, which is known as the time of minimum spread. We can show that

$$(\Delta x)^2_t = (\Delta x)^2_{t_1} + \frac{2}{m} E_d (t-t_1)^2$$

by using the time dependence equation for the free particle derived earlier.

Uncertainty Relation and Minimizing Wave Packet

The spread $(\Delta A)^2$ of an operator A on a given wave packet is defined by $(\Delta A)^2 = \langle (A-\langle A\rangle)^2\rangle$. From this we can state an important theorem about Hermitian operators.

Theorem: (Uncertainty Relations).

Suppose A and B are Hermitian operators and $[A,B] = AB-BA = iC$. Then $\Delta A\, \Delta B \geq \frac{1}{2} |\langle C\rangle|$.

Proof: (1) We first show $\frac{1}{2} \langle C\rangle = \mathrm{Im} \langle AB\rangle$. Since $AB-BA = iC$ we have $\langle AB\rangle - \langle BA\rangle = i\langle C\rangle$. Also $\langle AB\rangle = (\psi,AB\psi) = (A\psi,B\psi) = (BA\psi,\psi) = (\psi,BA\psi)^* = \langle BA\rangle^*$. Hence $\langle AB\rangle - \langle BA\rangle = 2i\mathrm{Im} \langle AB\rangle = i\langle C\rangle$ proving (1).

(2) Let $\alpha = A - \langle A\rangle$ and $\beta = B - \langle B\rangle$. Then α and β are Hermitian and moreover $(\Delta A)^2 = \langle \alpha^2\rangle = \langle A^2\rangle - \langle A\rangle^2$ and $(\Delta B)^2 = \langle \beta^2\rangle = \langle B^2\rangle - \langle B\rangle^2$. Then

$$(\Delta A)^2(\Delta B)^2 = \langle\alpha^2\rangle\langle\beta^2\rangle = (\psi,\alpha^2\psi)(\psi,\beta^2\psi) = (\alpha\psi,\alpha\psi)(\beta\psi,\beta\psi)$$

$$= ||\alpha\psi||^2\ ||\beta\psi||^2 \geq |(\alpha\psi,\beta\psi)|^2 .$$

Hence $\Delta A\, \Delta B \geq |(\alpha\psi,\beta\psi)| = |(\psi,\alpha\beta\psi)| = |\langle\alpha\beta\rangle|$. Then

$$\alpha\beta = (A-\langle A\rangle)(B-\langle B\rangle) = AB - \langle A\rangle B - \langle B\rangle A + \langle A\rangle\langle B\rangle ,$$

and so

$$\langle\alpha\beta\rangle = \langle AB\rangle - \langle A\rangle\langle B\rangle - \langle A\rangle\langle B\rangle + \langle A\rangle\langle B\rangle = \langle AB\rangle - \langle A\rangle\langle B\rangle .$$

But

$$\Delta A\ \Delta B \geq |\langle\alpha\beta\rangle| = |\langle AB\rangle - \langle A\rangle\langle B\rangle| \geq |\mathrm{Im}(\langle AB\rangle) - \mathrm{Im}(\langle A\rangle\langle B\rangle)|$$

$$= |\mathrm{Im}\langle AB\rangle| \ ,$$

since A,B Hermitian imply $\langle A\rangle$, $\langle B\rangle$ real. Since

$$|\mathrm{Im}\langle AB\rangle| = |\tfrac{1}{2}\langle C\rangle| = \tfrac{1}{2}|\langle C\rangle| \ ,$$

we obtain $\Delta A\ \Delta B \geq \frac{1}{2}|\langle C\rangle|$.

We observe that the equality $\Delta A\ \Delta B = \frac{1}{2}|\langle C\rangle|$ holds if and only if the following two conditions hold:

(1) $\alpha\psi$ and $\beta\psi$ are scalar multiples of one another,

(2) $\mathrm{Re}\langle AB\rangle = \langle A\rangle\langle B\rangle$.

We can apply the theorem to the product $\Delta x\ \Delta p$. Considering the momentum wavefunction $\phi(k)$ at fixed time, we have that the operators $x = i\hbar\frac{\partial}{\partial p} = i\frac{\partial}{\partial k}$ and $p = \hbar k$ are Hermitian, and $[x,p]\phi = i\hbar\frac{\partial}{\partial p}(p\phi) - p i\hbar\frac{\partial}{\partial p}(\phi) = i\hbar\phi$, so we have the operator equivalence $[x,p] = i\hbar$. By the theorem, $\Delta x\ \Delta p \geq \frac{\hbar}{2}$. To minimize the uncertainty product we require that $(x-\langle x\rangle)\phi$ and $(p-\langle p\rangle)\phi$ be scalar multiples, and $\mathrm{Re}\langle xp\rangle = \langle x\rangle\langle p\rangle$. Hence to minimize $\Delta x\ \Delta p$, $\phi(k)$ must satisfy $i\frac{\partial}{\partial k}\phi(k) - \langle x\rangle\phi(k) = \gamma[(\hbar k - p_0)\phi(k)]$, for undetermined complex number γ . We ignore the t dependence of ϕ ; $\Delta p\ \Delta x$ spreads out to become larger at all future and past time and we assume $t = t_1$ is the time of minimum $(\Delta x)^2$. Solving the differential equation gives

$$\phi(k) = N\, e^{-i([\langle x\rangle - \gamma p_0]k + \gamma\hbar\frac{k^2}{2})} \ .$$

for a normalization constant N such that $\int_{-\infty}^{\infty} |\phi(k)|^2 \, dk = 1$. This implies $\mathrm{Im}\, \gamma < 0$. In addition, ϕ must satisfy a number of other conditions namely

$$\int_{-\infty}^{\infty} \phi^*(k) \left(i \frac{\partial}{\partial k}\right) \phi(k) \, dk = \langle x \rangle \quad ,$$

and

$$\int_{-\infty}^{\infty} \phi^*(k) \, \hbar k \, \phi(k) dk = p_0 \quad .$$

If we write $\gamma = \alpha - i\beta$ where $\beta > 0$, then ϕ becomes

$$\phi(k) = N \, e^{\frac{\beta \hbar k_0^2}{2}} \, e^{-i[\frac{\alpha \hbar k^2}{2} + \langle x \rangle k - p_0 \, \alpha k]} \, e^{-\beta \frac{\hbar}{2}(k-k_0)^2} \quad ,$$

where $p_0 = \hbar k_0$.

Applying the normalization condition we obtain $N = \sqrt[4]{\frac{\beta \hbar}{\pi}} \, e^{-\beta \hbar k_0^2/2}$. Hence

$$\phi(k) = \sqrt[4]{\frac{\beta \hbar}{\pi}} \, e^{-i[\frac{\alpha \hbar k^2}{2} + \langle x \rangle k - p_0 \, \alpha k]} \, e^{-\frac{\beta \hbar}{2} (k-k_0)^2} \quad .$$

We now apply the condition $\int_{-\infty}^{\infty} \phi^*(k) \, \hbar k \, \phi(k) dk = p_0 = \hbar k_0$. An integration proves that is is automatically satisfied. Consider

$$\int_{-\infty}^{\infty} \phi^*(k) \left(i \frac{\partial}{\partial k}\right) \phi(k) \, dk \quad .$$

But $i \frac{\partial}{\partial k} \phi(k) = (\langle x \rangle + \gamma \hbar k - \gamma p_0) \, \phi(k)$ so $\int_{-\infty}^{\infty} \phi^*(k) (i \frac{\partial}{\partial k}) \phi(k) dk = \langle x \rangle$

follows immediately from $p_0 = <\hbar k>$. We now consider the final condition for ϕ namely $\mathrm{Re}\,<xp> = <x>\,p_0$.

$$<xp> = \int_{-\infty}^{\infty} \phi^*(k)\left(i\frac{\partial}{\partial k}\right)[\hbar k\,\phi(k)]dk = i\hbar + i\hbar\int \phi^*(k)\,k\,\frac{\partial}{\partial k}\phi(k)\,dk$$

$$= i\hbar + \hbar\int \phi^*(k)\,k\left[i\frac{\partial}{\partial k}\phi(k)\right]dk = i\hbar + \hbar[<k><x> - <k>\gamma p_0 + \gamma\hbar<k^2>] \ .$$

We note $<k^2> = k_0^2 + \frac{1}{2\beta\hbar}$, so

$$<xp> = i\hbar + p_0<x> - \gamma p_0^2 + \gamma\hbar^2\left[k_0^2 + \frac{1}{2\beta\hbar}\right] = i\hbar + p_0<x> + \frac{\gamma\hbar}{2\beta} \ .$$

Hence $\mathrm{Re}<xp> = p_0<x> + \frac{\alpha\hbar}{2\beta}$. The condition $\mathrm{Re}<xp> = <x>\,p_0$ implies $\alpha = 0$. Hence ϕ becomes

$$\phi(k) = \sqrt[4]{\frac{\beta\hbar}{\pi}}\, e^{-i<x>k}\, e^{-\frac{\beta\hbar}{2}(k-k_0)^2} \ . \qquad (6)$$

Equation (6) is the form of $\phi(k)$ which minimizes the uncertainty product $\Delta x\,\Delta p$. Since $\Delta x\,\Delta p$ is minimized at time $t = t_1$, (6) represents $\phi(k,t_1)$. Using (3) we obtain

$$\phi(k,t) = \sqrt[4]{\frac{\beta\hbar}{\pi}}\, e^{-i<x>_{t_1}k}\, e^{-\frac{\beta\hbar}{2}(k-k_0)^2}\, e^{-\frac{i\hbar k^2}{2m}(t-t_1)}$$

$$= \sqrt[4]{\frac{\beta\hbar}{\pi}}\, e^{-ik\left[\frac{<x>_{t_1} + <x>_t}{2}\right]}\, e^{-\frac{\beta\hbar}{2}(k-k_0)^2}\, e^{-\frac{i\hbar k(k-k_0)}{2m}(t-t_1)} \ .$$

We have used $<x>_t = <x>_{t_1} + (t-t_1)v$, $v = \frac{p_0}{m} = \frac{\hbar k_0}{m}$.

Equation (6) gives the momentum wave function at time t_1, namely

$$\phi(k,t_1) = \sqrt[4]{\frac{\beta\hbar}{\pi}}\, e^{-i\langle x\rangle k}\, e^{-\frac{\beta\hbar}{2}(k-k_0)^2} .$$

The position wave function is determined by Fourier Transformation to be

$$\psi(x,t_1) = \psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{ikx}\, dk \quad , \text{ or}$$

$$\psi(x) = \frac{1}{\sqrt[4]{\beta\hbar\pi}} \exp(ik_0(x-\langle x\rangle)) \exp\left(\frac{-(x-\langle x\rangle)^2}{2\beta\hbar}\right) . \qquad (7)$$

The constant $\beta > 0$ is related to the stationary energy E_d. Recall $E = E_d + E_t$ where $E_t = \frac{p_0^2}{2m} = \frac{\hbar^2 k_0^2}{2m}$. We have

$$E_d = \frac{\hbar^2}{4m\beta} . \qquad (8)$$

Recall $\frac{(\Delta k)^2\hbar^2}{2m} = E - \frac{p_0^2}{2m} = E_d$. Hence $\Delta k = \frac{1}{\sqrt{2\hbar\beta}}$. Since for a minimizing wavefunction $\Delta k\, \Delta x = \frac{1}{2}$, we have $\Delta x = \sqrt{\frac{\hbar\beta}{2}}$. Hence the parameter β determines the stationary energy and the spread of position and momentum. We observe that as time t differs from t_1, Δk will remain constant at $\frac{1}{\sqrt{2\hbar\beta}}$, but Δx will increase as previously determined which means

$$(\Delta x)_t^2 = \frac{\hbar\beta}{2} + \left(\frac{2E}{m} - \frac{p_0^2}{m^2}\right)(t-t_1)^2 = \frac{\hbar\beta}{2} + \frac{2E_d}{m}(t-t_1)^2 .$$

Hence,

$$(\Delta x)_t^2 = \frac{\hbar\beta}{2} + \frac{\hbar}{2m^2\beta}(t-t_1)^2 \quad \text{for} \quad \beta > 0 \ . \tag{9}$$

Equation (9) shows that for large β, the position wavefunction ψ has a large spread and its time dependence is slow. For small β the wavefunction ψ is very narrow at t_1, but spreads out rapidly.

We saw that the momentum wavefunction for the minimum uncertainty product packet was given by

$$\phi(k,t) = \sqrt[4]{\frac{\beta\hbar}{\pi}}\, e^{-i\langle x\rangle_{t_1} k}\, e^{-\frac{\beta\hbar}{2}(k-\langle k\rangle)^2}\, e^{-\frac{i\hbar k^2}{2m}(t-t_1)} \ ,$$

$$\phi(k,t) = \left(\frac{\beta\hbar}{\pi}\right)^{1/4} \exp\left[-i\langle x\rangle_{t_1} k - \frac{\beta\hbar}{2}(k-\langle k\rangle)^2 - \frac{i\hbar k^2}{2m}(t-t_1)\right] \ .$$

Here t_1 is the time of minimum spread Δx, $\langle k\rangle$ is the expected value of momentum and $\langle x\rangle_{t_1}$ is the expected value of position at time t_1. $\beta > 0$ is a real parameter designed to specify the relative amounts of position and momentum uncertainty.

The position wavefunctions $\psi(x,t)$ can be obtained in two ways:

(1) Fourier transform the expression for $\phi(k,t)$ above by taking

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k,t)\, e^{ikx}\, dk \ .$$

(2) Start with the expression for the position wavefunction at time t_1 namely

$$\psi(\bar{x},t_1) = (\beta\hbar\pi)^{-1/4} \exp\left[i\langle k\rangle(\bar{x} - \langle x\rangle_{t_1}) - \frac{(\bar{x}-\langle x\rangle_{t_1})^2}{2\beta\hbar}\right]$$

and use the general time dependence integral

$$\psi(x,t) = \frac{(1-i)}{2}\sqrt{\frac{m}{\pi\hbar(t-t_1)}}\int_{-\infty}^{\infty}\psi(\bar{x},t_1)\exp\left(\frac{im(x-\bar{x})^2}{2\hbar(t-t_1)}\right)d\bar{x} \quad .$$

In either case, the result turns out to be

$$\psi(x,t) = \left(\frac{\beta\hbar}{\pi}\right)^{1/4}\left(\beta\hbar+\frac{i\hbar}{m}(t-t_1)\right)^{-1/2}\exp\left(\frac{-\beta\hbar}{2}\langle k\rangle^2+\frac{(i[x-\langle x\rangle_{t_1}]+\beta\hbar\langle k\rangle)^2}{2[\beta\hbar+\frac{i\hbar}{m}(t-t_1)]}\right). \quad (10)$$

If we set $\langle x\rangle_{t_1} = 0$, $t_1 = 0$, $\langle k\rangle = 0$, $\beta = \frac{1}{\alpha\hbar}$ we can reduce this to equation (5), namely

$$\psi(x,t) = \left(\frac{\alpha}{\pi}\right)^{1/4}\left(1+\frac{i\hbar\alpha t}{m}\right)^{-1/2}\exp\left(\frac{-\alpha mx^2}{2[m+i\hbar\,\alpha t]}\right) \quad .$$

If we substitute $\beta\hbar = \frac{1}{2(\Delta k)^2}$ into (24) we have

$$\psi(x,t) = (2(\Delta k)^2\pi)^{-1/4}\left(\frac{1}{2(\Delta k)^2}+\frac{i\hbar}{m}(t-t_1)\right)^{-1/2}\exp\left(\frac{-\langle k\rangle^2}{4(\Delta k)^2}+\frac{(i[x-\langle x\rangle_{t_1}]+\frac{\langle k\rangle}{2(\Delta k)^2})^2}{2[\frac{1}{2(\Delta k)^2}+\frac{i\hbar}{m}(t-t_1)]}\right). \quad (11)$$

This gives the complete minimum uncertainty wavefunction in one dimension for the free particle in terms of

(1) t_1 the time of minimum spread,

(2) $\langle k\rangle$ the mean (average) or expected momentum (constant in time),

(3) $\langle x\rangle_{t_1}$ the expected position at time t_1 ,

(4) Δk the momentum spread (a constant in time).

The energy expectation is $E = \frac{\hbar^2(\langle k\rangle)^2}{2m} + E_d$ where $E_d = \frac{\hbar^2}{4m\beta} = \frac{\hbar^2\,\Delta k^2}{2m}$, meaning $E = \frac{\hbar^2}{2m}((\langle k\rangle)^2 + (\Delta k)^2)$.

The momentum wavefunction is

$$\phi(k,t) = (2\pi(\Delta k)^2)^{-1/4} \exp(-i\langle x\rangle_{t_1} k - \frac{(k-\langle k\rangle)^2}{4(\Delta k)^2} - \frac{i\hbar k^2}{2m}(t-t_1)) \quad . \qquad (12)$$

The position spread is (at time t)

$$(\Delta x)_t^2 = \frac{1}{4(\Delta k)^2} + \frac{\hbar^2(\Delta k)^2\,(t-t_1)^2}{2m^2} \quad .$$

The results in this section can easily be generalized to three dimensional cartesian coordinates. One dimension is used for economy of notion and simplicity.

CHAPTER II

TIME DELAY THEORY IN CLASSICAL MECHANICS

Consider a rolling frictionless ball in one dimension, with a height component y and a position component x in a gravitational field g. Suppose the ball has to pass over a hill $y = h(x)$ between $x = -a$ and $x = +a$.

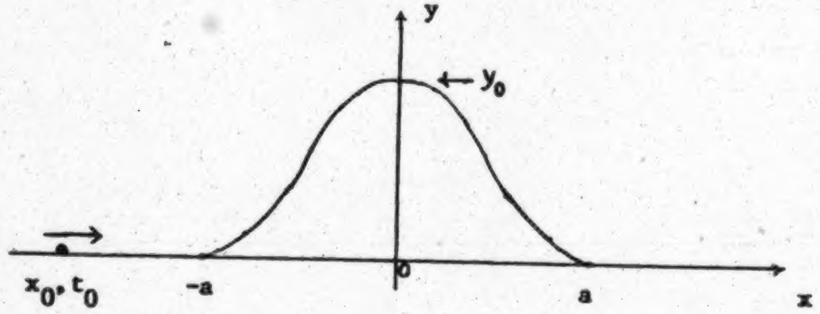

Figure 1

Classical Potential Hill

Assume the ball is a point mass and has no rotational kinetic energy. Assume that before interacting with the potential $V(x) = mgh(x)$ the ball is approaching the potential from the left with velocity v_0 where $\frac{1}{2} mv_0^2 > mgy_0$ where y_0 is the maximum of $h(x)$ for all x. Suppose that the ball has position x_0 at time t_0 where $x_0 < -a$.

The x and y components of the ball satisfy $y = h(x)$. Conservation of energy gives $\frac{1}{2} mv_0^2 = \frac{1}{2} m[(\frac{dx}{dt})^2 + (\frac{dy}{dt})^2] + mgy$, so

$$\frac{1}{2}mv_0^2 = \frac{1}{2}m(\dot{x}^2 + (h'(x)\dot{x})^2) + mgy$$

$$= \frac{1}{2}m\,\dot{x}^2(1 + h'^2(x)) + mgy \quad .$$

Hence

$$\frac{\frac{1}{2}mv_0^2 - mgh(x)}{1 + h'^2(x)} = \frac{1}{2}m\dot{x}^2 \quad \text{or} \quad \dot{x}^2 = \frac{v_0^2 - 2gh(x)}{1 + h'^2(x)} \quad .$$

Thus

$$\frac{dt}{dx} = \sqrt{\frac{1 + h'^2(x)}{v_0^2 - 2gh(x)}} \quad \text{so} \quad t = \int\sqrt{\frac{1 + h'^2(x)}{v_0^2 - 2gh(x)}}\,dx \quad .$$

Initial conditions t_0 , x_0 give us the relation

$$t = t_0 + \int_{x_0}\sqrt{\frac{1 + [h'(x)]^2}{v_0^2 - 2gh(x)}}\,dx \quad .$$

In particular, for $h(x) = 0$ we get the free particle equation $t' = t_0 + \dfrac{x - x_0}{v_0}$ for the one dimensional classical motion. The ' indicates this is undisturbed motion. The time delay $\Delta t = t - t'$ at the point x is given by

$$(\Delta t)_x = t-t' = \int_{x_0}\sqrt{\frac{1 + [h'(x)]^2}{v_0^2 - 2gh(x)}}\,dx - \frac{(x-x_0)}{v_0} \quad . \tag{1}$$

Now consider the particle in one dimension which is under the influence of a potential $V(x)$. Unlike the gravitational problem above, this is strictly one dimensional.

Assume that $V(x)$ is non-zero only for $-a \le x \le a$. Let $x_0 < -a$ and assume the particle is at x_0 at time t_0 and moving to the right. Conservation of energy gives us

$$\frac{1}{2} mv_0^2 = \frac{1}{2} m\dot{x}^2 + V(x) \text{ , so that } t = t_0 + \int_{x_0} \frac{dx}{\sqrt{v_0^2 - \frac{2}{m} V(x)}} \text{ .}$$

The time delay is

$$(\Delta t)_x = t - t' = \int_{x_0} \frac{dx}{\sqrt{v_0^2 - \frac{2}{m} V(x)}} - \frac{(x - x_0)}{v_0} \text{ .} \qquad (2)$$

The Three Parameter Potential

In order to determine what information time delay measurements give about a potential function we introduce a model potential $V(x)$ known as the three parameter poential. Results of measuring Δt aid us in obtaining the three parameters and consequently the form of the potential.

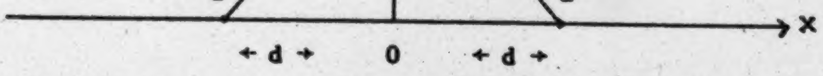

Figure 2

Piecewise Smooth Three Parameter Potential

$V(x)$ is assumed symmetric about $x = 0$. The potential acts between $-a$ and a where $a = w+d$. d , h and w are the three parameters needed to specify $V(x)$.

Let us calculate the time delay for the three parameter potential in the case of the particle under gravity. Substituting $h(x) = \frac{V(x)}{mg}$ in the expression for $(\Delta t)_x$ we get

$$(\Delta t)_x = \int_{x_0} \sqrt{\frac{1 + [V'(x)]^2/m^2g^2}{v_0^2 - \frac{2}{m}V(x)}}\,dx - \frac{(x-x_0)}{v_0} \quad .$$

Let us take $x_0 = -a = -w-d$ and $x = a = w+d$. The integration over x can be split into 3 intervals. The eventual result is

$$\Delta t = -2\left(\frac{w+d}{v_0}\right) + \frac{2w}{\sqrt{v_0^2 - \frac{2h}{m}}} + 2\sqrt{\frac{m^2d^2}{h^2} + \frac{1}{g^2}}\left[v_0 - \sqrt{v_0^2 - \frac{2h}{m}}\right] . \tag{3}$$

Δt is the time delay after a complete interaction with the three parameter potential. If we hold d and w fixed and calculate the limit of Δt as $h \to 0$, we see that $\Delta t \to 0$.

The time delay for the free particle in one dimension which interacts with the three parameter potential is

$$\Delta t = \frac{2w}{\sqrt{v_0^2 - \frac{2h}{m}}} - 2\left(\frac{w+d}{v_0}\right) + 2\,\frac{md}{h}\left[v_0 - \sqrt{v_0^2 - \frac{2h}{m}}\right] \quad . \tag{4}$$

This is the same result we obtain by letting $g \to \infty$ in (3). It corresponds to increasing gravitational strength g and decreasing height h so as to maintain the same function $V(x)$ for the potential.

The Smooth Three Parameter Potential

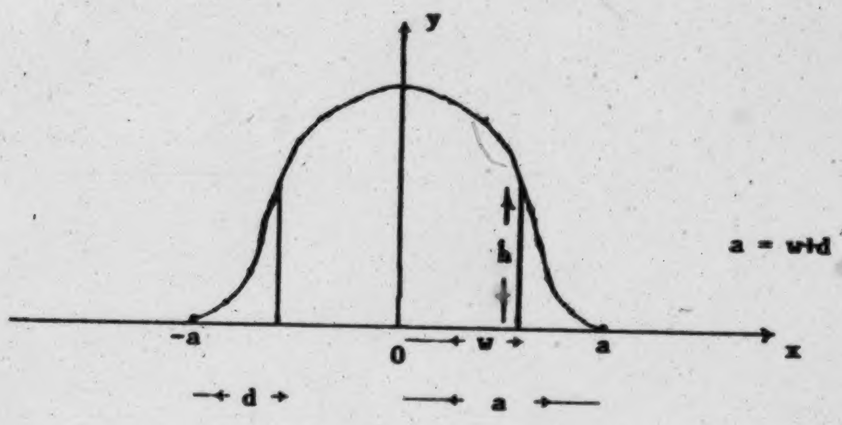

Figure 3

Smooth Three Parameter Potential

The smooth three parameter potential is a symmetric potential function constructed from parabolic arcs. On the interval $[w,a]$ on the x axis, $V(x)$ is the parabola passing through the points $(a,0)$ and (w,h) in the x-y plane which is tangent to the x axis at $x = a$. Similarly $V(x)$ is defined on $[-a,-w]$. On the interval $(-w,w)$ $V(x)$ is defined as a parabola that makes $V(x)$ and its derivative continuous at $\pm w$.

The explicit expression for $V(x)$ on each interval is

$$V(x) = \frac{h}{d^2}(x + w + d)^2 \quad \text{on} \quad [-w-d,-w] \;,$$

$$V(x) = h + \frac{wh}{d} - \frac{h}{dw}x^2 \quad \text{on} \quad [-w,w] \;, \qquad (5)$$

$$V(x) = \frac{h}{d^2}(x-w-d)^2 \quad \text{on} \quad [w,w+d] \;.$$

Let us determine the time delay Δt for the one dimensional interaction with the smooth three parameter potential. It is given by

$$\Delta t = \int_{-w-d}^{w+d} \frac{dx}{\sqrt{v_0^2 - \frac{2}{m} V(x)}} - \frac{2(w+d)}{v_0} ,$$

$$= 2 \int_{w}^{w+d} \frac{dx}{\sqrt{v_0^2 - \frac{2h}{md^2} (x-w-d)^2}} + \int_{-w}^{w} \frac{dx}{\sqrt{v_0^2 - \frac{2}{m} [h + \frac{wh}{d} - \frac{h}{dw} x^2]}} - \frac{2(w+d)}{v_0} .$$

We assume v_0 is large enough so that the argument of the square root is positive. The integral on the range $-w$ to w is symmetric about $x = 0$ and so

$$\Delta t = 2 \int_{w}^{w+d} \frac{dx}{\sqrt{v_0^2 - \frac{2h}{md^2} (x-w-d)^2}} + 2 \int_{0}^{w} \frac{dx}{\sqrt{v_0^2 - \frac{2}{m} [h + \frac{wh}{d} - \frac{h}{wd} x^2]}} - \frac{2(w+d)}{v_0} ,$$

$$\Delta t = 2d \sqrt{\frac{m}{2h}} \arcsin \left(\frac{\sqrt{\frac{2h}{m}}}{v_0} \right) + 2 \sqrt{\frac{mwd}{2h}} \sinh^{-1} \left(\frac{1}{\sqrt{\frac{md}{2wh} v_0^2 - \frac{d}{w} - 1}} \right) - \frac{2(w+d)}{v_0} . \quad (6)$$

One could curve fit equation (6) which describes Δt as a function of v_0 for $v_0^2 > \frac{2h}{m} + \frac{2wh}{md}$ to experimentally measured values of Δt in terms of v_0. This would give a means for determining the parameters w, d and h.

High Energy Approximations

For large v_0 satisfying $v_0^2 >> \frac{2h}{m} + \frac{2wh}{md}$ we can approximate in (6) above to get

$$\Delta t \simeq \frac{2hw}{md\, v_0^3} [d + \frac{2}{3} w] + \frac{2hd}{3m\, v_0^3} \quad . \tag{7}$$

Thus for high energy particles Δt is proportional to $\frac{1}{v_0^3}$ and the constant of proportionality, given in (7), is expressed in terms of the three parameters of the potential. This only gives us one equation for the three parameters, if we measure Δt for large v_0 and determine the coefficient. To get all three parameters we need three equations, and consequently it is necessary to expand Δt to a higher order. As an example let us take the piecewise smooth 3-parameter potential whose time delay for interaction is given by equation (4). Expanding in powers of v_0 we get

$$\Delta t \simeq \frac{(2w+d)h}{m\, v_0^3} + \frac{(3w+d)h^2}{m^2\, v_0^5} + \frac{(5w + \frac{5}{4} d)h^3}{m^3\, v_0^7} \quad .$$

By curve fitting this expression for large v_0 we get three coefficients, which lets us solve for the three parameters w , d and h .

In general, measurement of Δt as a function of v_0 determines some of the properties of the potential $V(x)$, but not the complete function V itself. The time delay is unchanged if the potential is displaced linearly along the x axis, or reflected through the y axis for instance.

Let us suppose that $V(x)$ is non-zero only for $-a \leq x \leq a$. The time delay for interaction is

$$\Delta t = \int_{-a}^{a} \frac{dx}{\sqrt{v_0^2 - \frac{2}{m} V(x)}} - \frac{2a}{v_0} \quad .$$

Suppose $v_0^2 >> \frac{2}{m} V(x)$ for all x in the interval $-a \leq x \leq a$. We write the integrand as

$$\begin{aligned}(v_0^2 - \frac{2}{m} V(x))^{-1/2} &= \frac{1}{v_0} (1 - \frac{2V(x)}{m\, v_0^2})^{-1/2} \\ &= \frac{1}{v_0} [1 + \sum_{n=1}^{\infty} \frac{(-1)^n\ (2n-1)!}{(n-1)!n!2^{2n-1}} (\frac{-2V(x)}{m\, v_0^2})^n] \quad , \\ &= \frac{1}{v_0} [1 + \sum_{n=1}^{\infty} \frac{(2n-1)!}{(n-1)!n!2^{n-1}} [\frac{V(x)}{m\, v_0^2}]^n] \quad .\end{aligned}$$

Let $V_n = \int_{-a}^{a} [V(x)]^n\, dx$. We get Δt expressed as

$$\Delta t = \sum_{n=1}^{\infty} \frac{(2n-1)!\ V_n}{(n-1)!n!\ 2^{n-1}\ m^n\ v_0^{2n+1}} \quad .$$

By measuring Δt as a function of v_0 we can determine the coefficients V_n which in turn give us information about V. The total information which time delay measurement gives us about the potential is the set of all coefficients V_n.

Hamiltonian Formulation

Consider the point mass in one dimension approaching a potential barrier $V(x)$ on $-a \leq x \leq a$, with sufficient energy to overcome it and pass through. The Hamiltonian function representing energy is $H = \frac{p^2}{2m} + V(x)$. The time function $\tau_0(t,p,x)$ is $\tau_0(t,p,x) = t + \tau(p,x)$ where $\{H,\tau\} = \frac{\partial H}{\partial x}\frac{\partial \tau}{\partial p} - \frac{\partial H}{\partial p}\frac{\partial \tau}{\partial x} = 1$. We take

$$\tau_0 = t - (\tfrac{m}{2})^{1/2} \int_{x_1}^{x} [\tfrac{p^2}{2m} + V(x) - V(\xi)]^{-1/2}\, d\xi \quad .$$

This means that $\tau(p,x) = -(\frac{m}{2})^{1/2} \int_{x_1}^{x} [\frac{p^2}{2m} + V(x) - V(\xi)]^{-1/2}\, d\xi$ and $\tau_0(t,p,x) = t + \tau(p,x)$. It is easy to see that τ satisfies $V'(x)\frac{\partial \tau}{\partial p} - \frac{p}{m}\frac{\partial \tau}{\partial x} = 1$ which is the conjugacy equation. (τ is conjugate to H.) We measure time t as $t = \tau_0 - \tau(p,x)$ where τ_0 is a constant. This gives us the time variation in terms of position x. The momentum p is always determined from x and is positive, so $p = \sqrt{2m(H-V(x))}$ as a function of x for constant H. Thus $t = \tau_0 - \tau(\sqrt{2m(H-V(x))}\, , x)$ gives the time t as a function of position x in terms of constant parameters τ_0 and H. Substituting explicitly for $\tau(p,x)$ we obtain

$$t = \tau_0 + (\tfrac{m}{2})^{1/2} \int_{x_1}^{x} [H - V(\xi)]^{-1/2}\, d\xi \quad .$$

In our original notation, $\tau_0 = t_0$, $x_1 = x_0$ and $H = \frac{1}{2} m v_0^2$. At time t_0 the particle was at position x_0 outside the potential range and had speed v_0 approaching the potential. We had the equation

$$t = t_0 + \int_{x_0} \frac{dx}{\sqrt{v_0^2 - \frac{2}{m} V(x)}}$$ from which we obtained equation (2).

We summarize the three parameter potentials as follows:

(a) Smooth three parameter potential.

$$V(x) = \frac{h}{d^2}(x + w + d)^2 \quad \text{for} \quad -w-d \le x \le -w \;,$$

$$V(x) = h + \frac{wh}{d} - \frac{h}{wd} x^2 \quad \text{for} \quad -w \le x \le w \;, \quad a = w+d \;,$$

$$V(x) = \frac{h}{d^2}(x - w - d)^2 \quad \text{for} \quad w \le x \le w+d \;.$$

(b) Piecewise smooth three paramter potential.

$$V(x) = \frac{h}{d}(x + d + w) \quad \text{for} \quad -w-d \le x \le -w \;,$$

$$V(x) = h \quad \text{for} \quad -w \le x \le w \;, \quad a = w+d \;,$$

$$V(x) = \frac{h}{d}(-x + d + w) \quad \text{for} \quad w \le x \le w+d \;.$$

(c) Piecewise constant three parameter potential.

$$V(x) = b \quad \text{for} \quad -2s \le x \le -s \;,$$

$$V(x) = h \quad \text{for} \quad -s \le x \le s \;, \quad a = 2s \;, \; b < h \;,$$

$$V(x) = b \quad \text{for} \quad s \le x \le 2s \;.$$

In each case (a), (b), (c) above, we can evaluate V_1, V_2, V_3 where

$V_n = \int_{-a}^{a} [V(x)]^n \, dx$ to get the results

$$\text{(a)} \quad V_n = 2\int_{w}^{w+d} [\frac{h}{d^2}(x-w-d)^2]^n \, dx + 2\int_{0}^{w} (h + \frac{wh}{d} - \frac{h}{wd}x^2)^n \, dx \quad ,$$

$$V_1 = \frac{2}{3} hd + 2hw + \frac{4}{3}\frac{w^2h}{d} \quad ,$$

$$V_2 = \frac{2h^2d}{5} + 2h^2w\,[1 + \frac{4w}{3d} + \frac{8w^2}{15d^2}] \quad ,$$

$$V_3 = \frac{2}{7} h^3d + 2h^3w\,[1 + \frac{2w}{d} + \frac{8}{5}\frac{w^2}{d^2} + \frac{16}{35}\frac{w^3}{d^3}] \quad ,$$

$$\text{(b)} \quad V_n = 2\int_{w}^{w+d} [\frac{h}{d}(-x+d+w)]^n dx + 2\int_{0}^{w} h^n \, dx \quad ,$$

$$V_1 = hd + 2hw \quad ,$$

$$V_2 = \frac{2}{3} h^2d + 2h^2w \quad ,$$

$$V_3 = h^3\frac{d}{2} + 2h^3w \quad ,$$

$$\text{(c)} \quad V_n = 2(h^n + b^n)s \quad , \quad (b < h) \quad .$$

The series for Δt expanded in the powers of $\frac{1}{v_0^3}$, $\frac{1}{v_0^5}$, $\frac{1}{v_0^7}$, etc. has the first three terms as

$$\Delta t = \frac{V_1}{m\,v_0^3} + \frac{3V_2}{2m^2\,v_0^5} + \frac{5V_3}{2m^3\,v_0^7} + \cdots \quad .$$

If we know Δt as a function of v_0 for large v_0 sufficiently well to determine the three parameters V_1, V_2, V_3, then the form of the potential can be determined according to (a), (b) or (c) above.

As an example, let us take case (b) and solve for w , h , d in terms of V_1 , V_2 , V_3 . We have

$$\frac{V_1}{h} = d + 2w \quad , \quad \frac{V_2}{h^2} = \frac{2}{3} d + 2w \quad , \quad \frac{V_3}{h^3} = \frac{d}{2} + 2w \quad .$$

Eliminating d and w we get $d = 2(\frac{V_1}{h} - \frac{V_3}{h^3}) = 3(\frac{V_1}{h} - \frac{V_2}{h^2})$ so that $V_1 h^2 - 3V_2 h + 2V_3 = 0$ so we can solve this quadratic and get $h = \frac{3V_2 \pm \sqrt{9V_2^2 - 8V_1 V_3}}{2V_1}$. Knowing h , w and d can be obtained as $d = 3(\frac{V_1}{h} - \frac{V_2}{h^2})$ and $w = \frac{1}{2} (\frac{V_1}{h} - d)$.

Determining the Potential $V(x)$ From the Integrals $V_n = \int_{-a}^{a} [V(x)]^n dx$.

We saw that time delay measurements in one dimension yielded the numbers V_n as the total available information about the potential $V(x)$. We shall see that V_n do not uniquely determine $V(x)$, but do uniquely determine another function $G(h)$ from which we can get all possible $V(x)$ with moments V_n . Conversely $G(h)$ itself determines the V_n . $G(h)$ is positive or zero for all h .

First of all, given $V(x)$ let us construct $G(h)$. This is done as follows.

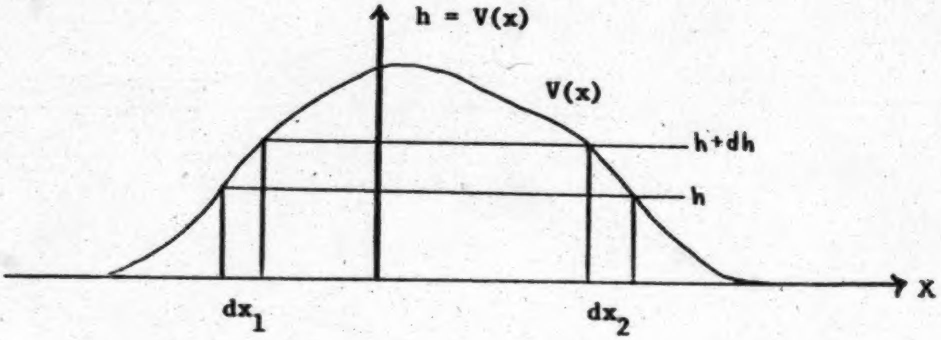

Figure 4

Constructing G(h)

Let $dx = |dx_1| + |dx_2|$ (both as positive values). Then $G(h) = \frac{dx}{dh}$. Also $V_n = \int_{-a}^{a} [V(x)]^n\, dx = \int_{V_{min}}^{V_{max}} h^n (\frac{dx}{dh})\, dh = \int_{V_{min}}^{V_{max}} h^n\, G(h)\, dh$. The equations $V_n = \int_{V_{min}}^{V_{max}} h^n\, G(h)\, dh$ determine G(h) , since it can be expanded in terms of orthogonal polynomials. If V(x) is monotone, $G(h) = \frac{1}{|V'(x)|}$ for h = V(x) . (Note $V_0 = 2a$.)

V_n tells us that given h , V(x) lies in the range h to h+dh for a given amount of interval width dx somewhere in [-a,a] . This interval width may be split into several pieces. $\frac{dx}{dh}$ is thus given in terms of h , and if the function V is symmetric about x = 0 (even function), one can uniquely determine V . Any function V(x) can be transformed into a symmetric one or monotone increasing one with all V_n unchanged. The V_n determines a symmetric or monotone V(x) uniquely up too total x translation. We observe that since

$V_n = \int_{-a}^{a} [V(x)]^n \, dx$, V_n cannot be specified arbitrarily. For instance $V_{2n} \geq 0$ and if $V(x) \geq 0$, $V_{2n+1} \geq 0$. In the equation $V_n = \int_{V_{min}}^{V_{max}} h^n G(h) \, dh$ we observe that $G(h) \geq 0$ and so $V_{2n} \geq 0$ and $V_{2n+1} \geq 0$ if $V(x) \geq 0$ so that $V_{min} \geq 0$.

Let us now suppose the potential $V(x)$ is an even function of x (symmetry about $x = 0$). Suppose also that the value of $V(0) = \alpha$. Then $V'(x) = \frac{dh}{dx_1} = \frac{dh}{\frac{1}{2} dx} = 2 \frac{dh}{dx} = \frac{2}{G(h)} = \frac{2}{G(V(x))} = \frac{d\,V(x)}{dx}$. Integrating gives $2x = \int_{\alpha}^{V(x)} G(y) \, dy$. This holds if $\alpha = V_{max}$ and $V(x)$ is monotone increasing on $[-a,0]$ and monotone decreasing on $[0,a]$. This gives x in terms of $V(x)$ for $x \in [-a,0]$, since $G(y) \geq 0$ and $V(x) \leq \alpha$. By symmetry we obtain x in terms of $V(x)$ for $x \in [0,a]$. In this particular case we can construct the unique symmetric even function, monotone increasing for negative x and decreasing for positive x in terms of the function $G(y)$. Observe that this is the form for all our three parameter potentials, and that it is uniquely determined by time delay measurements.

Since $V(x)$ is assumed to be of finite range $V(x) = 0$ for $x < -a$, $x > a$, we see that $V_{min} = 0$ and $V_{max} = V(0)$ for this special symmetric function. These are the consequences of assuming that $V(x)$ has a maximum and is symmetric about it. The monotone assumptions on $[-a,0]$ and $[0,a]$ make a single integration of $G(y)$ over y possible. This gives the basic reconstruction of $V(x)$ for a positive potential.

Let us consider one very special example of a one dimensional potential for which the time delay can be used to determine some of its properties.

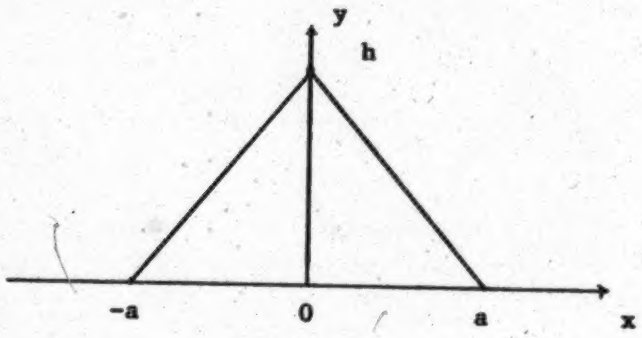

Figure 5

Triangular Potential

Define $V(x)$ to be zero for $x > a$ and $x < -a$. $V(x) = \frac{h}{a}x + h$ for $-a < x < 0$ and $V(x) = h - \frac{h}{a}x$ for $0 < x < a$. This is a form of the three parameter potential whose time delay is given by (4). We set $d = a$, $w = 0$ and $h = h$ to get

$$\Delta t = -\frac{2a}{v_0} + 2\,\frac{ma}{h}\,[v_0 - \sqrt{v_0^2 - \frac{2h}{m}}\,] \quad . \tag{8}$$

Now let us suppose we are given equation (8) describing Δt as a function of v_0 , and we know nothing about the potential $V(x)$. Expanding Δt as an infinite series in v_0 we get the following.

$$\Delta t = -\frac{2a}{v_0} + \frac{2ma\ v_0}{h}\left[1 - \sqrt{1 - \frac{2h}{m\,v_0^2}}\right] \ .$$

Now use the series $(1+x)^{1/2} = 1 + \frac{1}{2}x + \sum_{n=1}^{\infty} \frac{(-1)^n(2n-1)!x^{n+1}}{2^{2n}(n-1)!(n+1)!}$ and put $x = \frac{-2h}{m v_0^2}$ to get

$$\Delta t = \sum_{n=1}^{\infty} \frac{a(2n-1)!h^n}{2^{n-2}(n-1)!(n+1)!m^n v_0^{2n+1}} .$$

We compare this series expansion to the one for the general potential, namely

$$\Delta t = \sum_{n=1}^{\infty} \frac{(2n-1)!\, V_n}{(n-1)!n!2^{n-1} m^n v_0^{2n+1}} ,$$

and from this we conclude that $V_n = \frac{2ah^n}{n+1}$. V_n can be expressed as an integral of the function $G(y)$. We know the maximum height h from measurements of v_0 that fail to give transmission (or from (8) which implies $v_0^2 \geq \frac{2h}{m}$). This tells us that the maximum of $V(x)$ is h . For a positive potential, the minimum height is zero and so $V_n = \frac{2ah^n}{n+1} = \int_0^h y^n G(y)\, dy$. Without even expanding in orthogonal polynomials, we recognize immediately that $G(y) = \frac{2a}{h}$ a constant, independent of y .

If we assume that $V(x)$ is symmetric on $[-a,a]$ with maximum at $x = 0$, monotone increasing on $[-a,0]$ and decreasing on $[0,a]$ the form of $V(x)$ is uniquely determined by $G(y)$ to be the triangular function we started out with. However there are many more possible ways to construct non-symmetric $V(x)$ functions which still give the same time delay Δt . Some of these are

(1) $V(x) = \frac{hx}{2a}$ for $0 \leq x \leq 2a$, zero elsewhere.

(2)

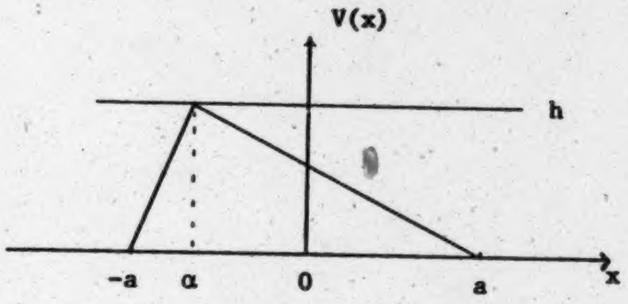

Figure 6

Non-symmetric Triangular Potentials

$$V(x) = \frac{h(x+a)}{\alpha+a} \quad \text{for} \quad -a < x < \alpha$$

$$V(x) = \frac{h(a-x)}{a-\alpha} \quad \text{for} \quad \alpha < x < a \quad .$$

(3) We know $G(y) = \frac{2a}{h} = \frac{dx}{dy}$ where $dx = |dx_1| + |dx_2|$. Since $|dx_1| + |dx_2| = \frac{2a}{h}\, dy$, let us choose $dx_1 = \frac{2a}{h}(1 - \frac{y}{h})\, dy$ and $-dx_2 = \frac{2a}{h}(\frac{y}{h})\, dy$. For boundary conditions, take $x_1 = x_2 = 0$ for $y = h$, and let $V(x_1) = y(x_1)$ for $x_1 < 0$ and $V(x_2) = y(x_2)$ for $x_2 > 0$. If we solve the equations by integrating we get

$$V(x) = h\left(1 - \sqrt{-\frac{x}{a}}\right) \quad \text{for} \quad -a < x \leq 0 \quad ,$$

$$= h\sqrt{1 - \frac{x}{a}} \quad \text{for} \quad 0 < x < a \quad .$$

In this case, the graph of $V(x)$ looks like the following.

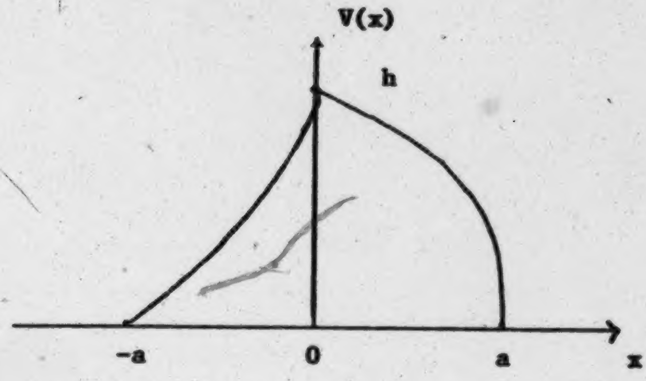

Figure 7

Curved Potential

CHAPTER III

SCATTERING FROM A CENTRAL POTENTIAL

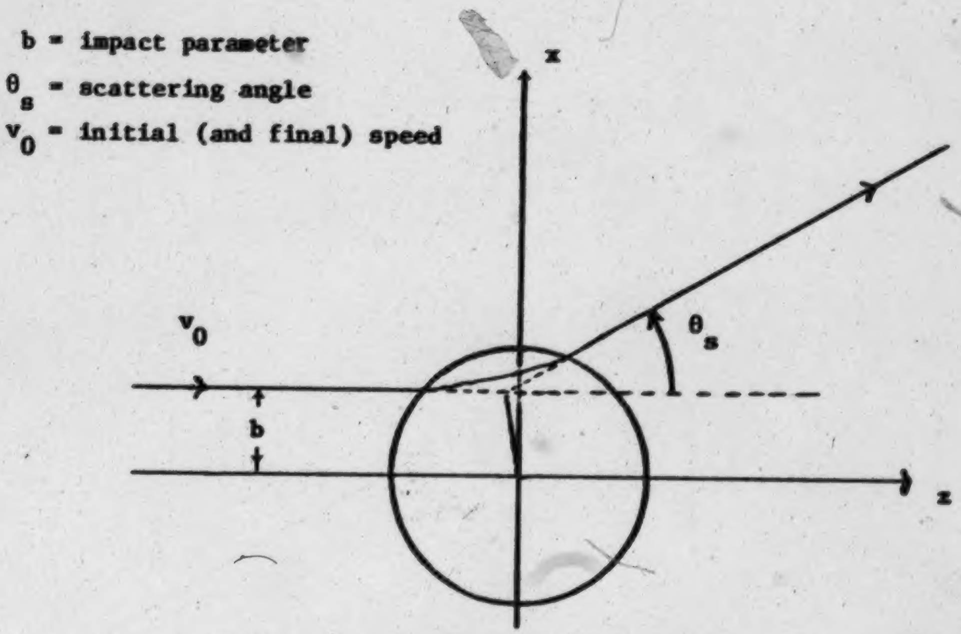
b = impact parameter
θ_s = scattering angle
v_0 = initial (and final) speed
x
v_0
θ_s
b
z

Figure 8

Central Potential Scattering

A three dimensional classical scattering problem with a potential $V(r)$ depending only on r, the distance from the origin, can be reduced to a two dimensional plane problem. Let $r^2 = x^2 + z^2$ and suppose $V(r)$ is non-zero only for $r < a$.

Let us represent the coordinates of the particle by r and θ where $z = r \cos \theta$, $x = r \sin \theta$. The Lagrangian expressed as a function of r, θ, $\dot{r}$, $\dot{\theta}$ is

$$L(r,\theta,\dot{r},\dot{\theta}) = \frac{1}{2}\, m(\dot{r}^2 + r^2\dot{\theta}^2) - V(r) \quad .$$

The equations of motion are $\frac{d}{dt}(\frac{\partial L}{\partial \dot{r}}) = \frac{\partial L}{\partial r}$ and $\frac{d}{dt}(\frac{\partial L}{\partial \dot{\theta}}) = \frac{\partial L}{\partial \theta} = 0$. These include conservation of energy and angular momentum. The conjugate momenta p_r and p_θ are

$$p_r = \frac{\partial L}{\partial \dot{r}} = m\dot{r} \quad \text{and} \quad p_\theta = \frac{\partial L}{\partial \dot{\theta}} = mr^2\,\dot{\theta} \quad .$$

Thus, the Hamiltonian is

$$H(r,\theta,p_r,p_\theta) = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + V(r) \quad .$$

The equations of motion are reformulated as $\frac{\partial H}{\partial p_r} = \dot{r}$, $\frac{\partial H}{\partial p_\theta} = \dot{\theta}$, $\frac{\partial H}{\partial r} = -\dot{p}_r$, $\frac{\partial H}{\partial \theta} = -\dot{p}_\theta$.

The motion of the particle is obtained by solving the equations $m\ddot{r} + V'(r) = mr\dot{\theta}^2$ and $mr^2\dot{\theta}$ = constant. The latter equation is conservation of angular momentum $(L = mr^2\dot{\theta})$. The first equation, $m\ddot{r} + V'(r) = \frac{L^2}{mr^3}$ can be solved by direct integration. Since $m\ddot{r} = \frac{L^2}{mr^3} - V'(r)$, $m(\frac{d\dot{r}}{dt})\dot{r}\, dt = [\frac{L^2}{mr^3} - V'(r)]\, dr$ and we integrate to get $\frac{1}{2}\, m\dot{r}^2 = -\frac{L^2}{2mr^2} - V(r)$ + constant. Thus $E = \frac{1}{2}\, m\dot{r}^2 + \frac{L^2}{2mr^2} + V(r)$ is a constant, and we have conservation of energy.

Suppose the particle is incident with velocity v_0 and impact parameter b . The two constants E and L of the motion are $E = \frac{1}{2}\, mv_0^2$ and $L = -mbv_0$. The E equation is $\frac{1}{2}\, mv_0^2 = \frac{1}{2}\, m\dot{r}^2 + \frac{L^2}{2mr^2} + V(r)$ and so

$$\frac{dr}{dt} = \pm \sqrt{v_0^2 - (\frac{L}{mr})^2 - \frac{2V(r)}{m}} = \pm \sqrt{v_0^2 \; [1 - \frac{b^2}{r^2}] - \frac{2}{m} V(r)} \quad .$$

r_{min} is the radius of closest approach. It satisfies $v_0^2 \; [1 - \frac{b^2}{r_{min}^2}] - \frac{2}{m} V(r_{min}) = 0$. Note that time measurement is made from the integral $t = \int \frac{dr}{\sqrt{v_0^2 \; [1 - \frac{b^2}{r^2}] - \frac{2}{m} V(r)}}$. The steps are

$$t_2 - t_1 = \int_{r_1}^{r_{min}} \frac{dr}{-\sqrt{v_0^2 \; [1 - \frac{b^2}{r^2}] - \frac{2}{m} V(r)}} + \int_{r_{min}}^{r_2} \frac{dr}{\sqrt{v_0^2 \; [1 - \frac{b^2}{r^2}] - \frac{2}{m} V(r)}} \; ,$$

so that

$$t_2 - t_1 = \Delta t = \int_{r_{min}}^{r_1} + \int_{r_{min}}^{r_2} \frac{dr}{\sqrt{v_0^2 \; [1 - \frac{b^2}{r^2}] - \frac{2}{m} V(r)}}$$

where t_1 is a time before scattering with $r = r_1$, and t_2 is a time after scattering with $r = r_2$.

The Scattering Angle θ_s .

The integration also provides a means for obtaining θ .

$$d\theta = - \frac{b v_0 dt}{r^2} = - \frac{b \; v_0 \; dr}{r^2 \sqrt{v_0^2 \; [1 - \frac{b^2}{r^2}] - \frac{2}{m} V(r)}} \quad .$$

Thus

$$\theta_2-\theta_1 = \Delta\theta = -bv_0 \int_{r_{min}}^{r_1} + \int_{r_{min}}^{r_2} \frac{dr}{r^2\sqrt{v_0^2\ [1 - \frac{b^2}{r^2}] - \frac{2}{m}\, V(r)}} \quad .$$

In particular $\Delta\,\theta < 0$ if $b > 0$. Also $\theta_s - \Delta\theta = \pi$ if we run the r limits to infinity. Therefore

$$\theta_s = \pi - 2bv_0 \int_{r_{min}}^{\infty} \frac{dr}{r^2\sqrt{v_0^2\ [1 - \frac{b^2}{r^2}] - \frac{2}{m}\, V(r)}} \quad . \qquad (1)$$

For example, if we take $r_{min} = b$ and $V(r) = 0$ we get $\theta_s = 0$. Equation (1) can be reformulated as an integral over $u = \frac{1}{r}$.

$$\theta_s = \pi - 2bv_0 \int_0^{1/r_{min}} \frac{du}{\sqrt{v_0^2[1 - b^2u^2] - \frac{2}{m}\, V(\frac{1}{u})}} \quad . \qquad (1)(a)$$

Time Delay in Scattering

In computing time delay, we assume that hard sphere interaction has zero time delay and so

$$\delta t = 2 \int_{r_{min}}^{\infty} \left[\frac{1}{\sqrt{v_0^2[1 - \frac{b^2}{r^2}] - \frac{2}{m}\, V(r)}} - \frac{1}{\sqrt{v_0^2[1 - \frac{b^2}{r^2}]}} \right] dr \quad . \qquad (2)$$

Unlike the one dimensional case we cannot hope to expand in an infinite series and isolate the dependence on v_0 or b, since the expansion coefficients are integrals, and in this case the integrals have r_{min} as a limit of integration. r_{min} has a complex dependence on v_0, b and the unknown potential $V(r)$.

A Model 4 Parameter Potential

One way to solve this problem is to construct the most general potential $V(r)$ for which the integrals in equations (1) and (2) can be analytically evaluated in terms of well known functions. To do this we define $V(r)$ as follows.

$$\begin{aligned} V(r) &= \alpha + \frac{\beta}{r} + \frac{\gamma}{r^2} \quad \text{for} \quad 0 \le r \le a \\ V(r) &= 0 \quad\quad\quad\quad\quad \text{for} \quad r > a \quad . \end{aligned} \tag{3}$$

The four parameters for this potential are α, β, γ, and a. Let us assume that the particle interacts with the potential (i.e., $r_{min} < a$). We do not consider the case of a miss ($r_{min} = b > a$) or a hard sphere reflection ($r_{min} = a \ge b$) in the case that V is discontinuous at a. For a miss, θ_s and δt are both zero. For hard sphere interaction, $\delta t = 0$ and θ_s can be calculated from simple geometrical concepts. For a hard sphere of radius a [$V(r) = 0$, $r > a$; $V(r) = +\infty$, $r < a$] we have $\theta_s = 2 \arccos \frac{b}{a}$. This result can also be obtained by setting $r_{min} = a$ and $V(r) = 0$ in (1).

The conditions required for interaction with the potential is $r_{min} < a$. This implies as a necessary condition $b < a$. Since the potential $V(r)$ may be discontinuous at $r = a$ we require also $v_0^2 [1 - \frac{b^2}{a^2}] > \frac{2}{m} V(a^+)$. Assuming potential interaction, let us determine r_{min} . It satisfies $\frac{m}{2} v_0^2 [1 - \frac{b^2}{r_{min}^2}] = v(r_{min}) = \alpha + \frac{\beta}{r_{min}} + \frac{\gamma}{r_{min}^2}$. This gives a quadratic for r_{min} , namely $(\frac{m}{2} v_0^2 - \alpha) r_{min}^2 - \beta\, r_{min} - (\gamma + \frac{mb^2}{2} v_0^2) = 0$. Thus

$$r_{min} = \frac{\beta \pm \sqrt{\beta^2 + 4(\frac{m}{2} v_0^2 - \alpha)(\gamma + \frac{mb^2}{2} v_0^2)}}{2(\frac{m}{2} v_0^2 - \alpha)} .$$

For v_0 large we see the + sign is the only one acceptable and

$$r_{min} = \frac{\beta + \sqrt{\beta^2 + (mv_0^2 - 2\alpha)(2\gamma + mb^2 v_0^2)}}{mv_0^2 - 2\alpha} . \qquad (4)$$

The Scattering Angle θ_s .

By equation (1)(a)

$$\theta_s = \pi - 2bv_0 \int_0^{1/r_{min}} \frac{du}{\sqrt{v_0^2[1 - b^2u^2] - \frac{2}{m} V(\frac{1}{u})}}$$

$$= \pi - 2bv_0 \int_0^{1/a} \frac{du}{v_0 \sqrt{1 - b^2u^2}} - 2bv_0 \int_{1/a}^{1/r_{min}} \frac{du}{\sqrt{v_0^2[1-b^2u^2] - \frac{2}{m}(\alpha+\beta u+\gamma u^2)}} .$$

For a positive potential we have $a > r_{min} > b$ in general. At the limit $\frac{1}{r_{min}}$ the denominator of the last integrand becomes zero. The result is

$$\theta_s = 2 \arccos \left(\frac{b}{a}\right) - \frac{2bv_0}{\sqrt{v_0^2 b^2 + \frac{2}{m}\gamma}} \arccos \left(\frac{\frac{v_0^2 b^2 + \frac{2\gamma}{m}}{a} + \frac{\beta}{m}}{\sqrt{(v_0^2 - \frac{2}{m}\alpha)(v_0^2 b^2 + \frac{2}{m}\gamma) + \frac{\beta^2}{m^2}}} \right) .$$

Example: Coulomb potential $V(r) = \frac{e^2}{r}$. Let $a \to \infty$ and set $\alpha = \gamma = 0$ and $\beta = e^2$ to get

$$\theta_s = 2 \arcsin \frac{1}{\sqrt{1 + v_0^4 b^2 \frac{m^2}{e^4}}} .$$

This is a very simple function of $v_0^2 b$ which can be checked by experiment. The potential given in equation (3) has the advantage of covering a wide range of possible potentials and yet it can still be evaluated in closed form. Expressed in terms of inverse tangent, $\theta_2 = 2 \arctan \left(\frac{e^2}{v_0^2 \, bm}\right)$ for the Coulomb potential.

Time Delay and True Time Delay

In addition to the time delay δt as defined in equation (2) we have another concept, that of true time delay, denoted by Δt . In terms of δt , Δt is given by

$$\Delta t = \delta t - 2 \int_{r_o}^{r_{min}} \frac{dr}{v_0 \sqrt{1 - \frac{b^2}{r^2}}} .$$

r_0 is less than r_{min} and is the radius of closest approach for hard sphere scattering that gives the same scattering angle θ_s as that for the potential. i.e., $r_0 = b \sec(\theta_s/2)$. Thus $b < r_0 < r_{min} < a$.

Consider now time delay for the potential defined by (3). From equation (2),

$$\delta(t) = 2\int_{r_{min}}^{a} \frac{dr}{\sqrt{v_0^2[1 - \frac{b^2}{r^2}] - \frac{2}{m}[\alpha + \frac{\beta}{r} + \frac{\gamma}{r^2}]}} - 2\int_{r_{min}}^{a} \frac{dr}{v_0\sqrt{1 - \frac{b^2}{r^2}}} .$$

Observe that the denominator of the first integrand is zero at the limit r_{min}. The result is

$$\delta t = \frac{2}{v_0^2 - \frac{2}{m}\alpha}\left[a^2(v_0^2 - \frac{2}{m}\alpha) - \frac{2a\beta}{m} - v_0^2\, b^2 - \frac{2\gamma}{m}\right]^{1/2}$$

$$+ \frac{2\beta}{m(v_0^2 - \frac{2}{m}\alpha)^{3/2}} \cosh^{-1}\left(\frac{a(v_0^2 - \frac{2}{m}\alpha) - \frac{\beta}{m}}{\sqrt{(v_0^2 b^2 + \frac{2\gamma}{m})(v_0^2 - \frac{2}{m}\alpha) + \frac{\beta^2}{m^2}}}\right) \qquad (6)$$

$$- \frac{2}{v_0}\left[\sqrt{a^2 - b^2} - \sqrt{r_{min}^2 - b^2}\right] .$$

Also we note that $\Delta t = \delta t - \frac{2}{v_0}\left[\sqrt{r_{min}^2 - b^2} - \sqrt{r_0^2 - b^2}\right]$. We see that $\sqrt{r_0^2 - b^2} = b \tan(\frac{\theta_s}{2})$ where θ_s is given by (5). Let us consider expanding θ_s and δt in powers of v_0 for large v_0. For large v_0, θ_s has a coefficient in $\frac{1}{v_0^2}$ as its dominating term. In this approximation

$$\theta_s \doteq \frac{2[\gamma + a\beta + \alpha b^2]}{\sqrt{a^2-b^2}\,(bmv_0^2)} + \frac{2\gamma}{mv_0^2\, b^2} \arccos\left(\frac{b}{a}\right) \quad . \tag{7}$$

By observing the high evergy $\frac{1}{v_0^2}$ dependence of θ_s as a function of $|b$ we may be able to determine the parameters α , β , γ , a of the potential. This only holds for b not too close to zero and v_0 large enough to make θ_s relatively small.

Let us consider now the high energy behavior of δt and Δt . We expect the high energy term to be of the form $\frac{1}{v_0^3}$. The highest terms in δt are

$$\delta t \simeq \frac{4\alpha\sqrt{a^2-b^2}}{m\, v_0^3} - \frac{2(a^2\alpha + a\beta + \gamma)}{m\, v_0^3 \sqrt{a^2-b^2}} + \frac{2\beta}{mv_0^3} \cosh^{-1}\left(\frac{a}{b}\right) + \frac{2}{v_0^2}\sqrt{\frac{2}{m}}\sqrt{b^2\alpha + b\beta + \gamma} \; .$$

The last term has $\frac{1}{v_0^2}$ dependence and indicates that Δt and not δt is the correct quantity for time delay measurement. The leading term in Δt is proportional to $\frac{1}{v_0^3}$ and so for large v_0

$$\Delta t \doteq \frac{4\alpha\sqrt{a^2-b^2}}{m\, v_0^3} - \frac{2(a^2\alpha + a\beta + \gamma)}{mv_0^3 \sqrt{a^2 - b^2}} + \frac{2\beta}{mv_0^3} \cosh^{-1}\left(\frac{a}{b}\right)$$

$$+ \frac{2[\gamma + a\beta + \alpha b^2]}{\sqrt{a^2-b^2}\; m\, v_0^3} + \frac{2\gamma}{mbv_0^3} \arccos\left(\frac{b}{a}\right) \quad . \tag{8}$$

Time delay as measured by Δt indicates the time difference between scattering off the given potential and a hard sphere with the same v_0 , b and θ_s . Time delay as measured by δt is time difference between scattering from the given potential and hard sphere for the same v_0 , b and r_{min} .

We can introduce a new time delay concept, that of impact parameter time delay defined by

$$\partial t = \Delta t - 2\int_b^{r_o} \frac{dr}{v_o\sqrt{1-\frac{b^2}{r^2}}} ,$$

$$= \delta t - 2\int_b^{r_{min}} \frac{dr}{v_o\sqrt{1-\frac{b^2}{r^2}}} .$$

It represents the time delay between actual scattering and no scattering at all.

Define $\partial_R t = 2\int_{r_{min}}^{R} \frac{dr}{\sqrt{v_0^2\,(1-\frac{b^2}{r^2}) - \frac{2}{m}V(r)}} - 2\int_b^R \frac{dr}{v_0\sqrt{1-\frac{b^2}{r^2}}}$.

Then $\partial_R t \to \partial t$ as $R \to \infty$. In fact if $V(r) = 0$ for $r > A$, then $\partial_R t = \partial t$ for $R > A$. Let us suppose that the potential $V(r)$ has range A . Then

$$\partial t = 2\int_{r_{min}}^{A} \frac{dr}{\sqrt{v_0^2\,(1-\frac{b^2}{r^2}) - \frac{2}{m}V(r)}} - 2\int_b^A \frac{dr}{v_0\sqrt{1-\frac{b^2}{r^2}}} ,$$

$$= \frac{2}{v_0}\int_{r_{min}}^{A} \frac{r\,dr}{\sqrt{[a(r)]^2 - b^2}} - \frac{2}{v_0}\int_b^A \frac{r\,dr}{\sqrt{r^2 - b^2}} ,$$

where $a(r) = r\sqrt{1 - \frac{2}{m\,v_0^2}V(r)}$. Hence

$$\partial_t(b,v_0) + \frac{2}{v_0}\int_b^A \frac{r\,dr}{\sqrt{r^2 - b^2}} = \frac{2}{v_0}\int_{r_{\min}}^A \frac{r\,dr}{\sqrt{[a(r)]^2 - b^2}} \ .$$

Observe that $a(r_{\min}) = b$. Thus $r_{\min} = a^{-1}(b)$ [inverse function]. Hence

$$\partial_t(b,v_0) + \frac{2}{v_0}\int_b^A \frac{r\,dr}{\sqrt{r^2 - b^2}} = \frac{2}{v_0}\int_{a^{-1}(b)}^A \frac{r\,dr}{\sqrt{[a(r)]^2 - b^2}} \ .$$

We can change the variable of integration in the last integral from r to $u = a(r)$. This gives us

$$\partial_t(b,v_0) + \frac{2}{v_0}\int_b^A \frac{r\,dr}{\sqrt{r^2 - b^2}} = \frac{2}{v_0}\int_b^{a(A)} \frac{a^{-1}(u)a^{-1'}(u)du}{\sqrt{u^2 - b^2}}$$

$$= \frac{2}{v_0}\int_b^A \frac{a^{-1}(u)a^{-1'}(u)du}{\sqrt{u^2 - b^2}} \ ,$$

using $a(A) = A$ since $V(A) = 0$. Changing the r integration to u integration in the integral on the other side and bringing it over we get

$$\partial_t(b,v_0) = \frac{2}{v_0}\int_b^A \frac{[a^{-1}(u)a^{-1'}(u)-u]du}{\sqrt{u^2 - b^2}} = \frac{2}{v_0}\int_b^A \frac{\gamma(u)\,du}{\sqrt{u^2 - b^2}}$$

where $\gamma(u) = a^{-1}(u)a^{-1'}(u) - u$. We assume v_0 is constant and b is varied. For each v_0 we have a different function $\gamma(u)$.

If $u > A$ we can see that $\gamma(u) = 0$ since $V(u) = 0$ so $a(u) = u$ and $a^{-1}(u) = u$ so $a^{-1'}(u) = 1$. Thus we may extend the above integral beyond A to ∞ as

$\partial_t(b,v_0) = \frac{2}{v_0}\int_b^\infty \frac{\gamma(u)\,du}{\sqrt{u^2 - b^2}}$, where $\gamma(u) = \gamma_{v_0}(u)$ depends on v_0 . We set $u^2 = s$ and $\beta = b^2$ and transform this integral to $g(\beta) = \int_\beta^\infty \frac{h(s)\,ds}{\sqrt{s-\beta}}$, where $g(\beta) = \partial_t(\beta^{1/2},v_0)$ and $h(s) = \frac{\gamma(s^{1/2})}{v_0 s^{1/2}}$. Let us experiment with $g(\beta) = \int_\beta^\infty \frac{h(s)\,ds}{\sqrt{s-\beta}}$. Multiply by $\frac{d\beta}{\sqrt{\beta-w}}$ and integrate from w to ∞ . We get

$$\int_w^\infty \frac{g(\beta)\,d\beta}{\sqrt{\beta-w}} = \int_{\beta=w}^\infty \frac{d\beta}{\sqrt{\beta-w}} \left(\int_{s=\beta}^\infty \frac{h(s)\,ds}{\sqrt{s-\beta}}\right) ,$$

$$= \int_{\substack{\text{Region } R\\ \text{in } s\beta \text{ plane}}} \left(\frac{h(s)}{\sqrt{\beta-w}\,\sqrt{s-\beta}}\right) d\beta\,ds \quad .$$

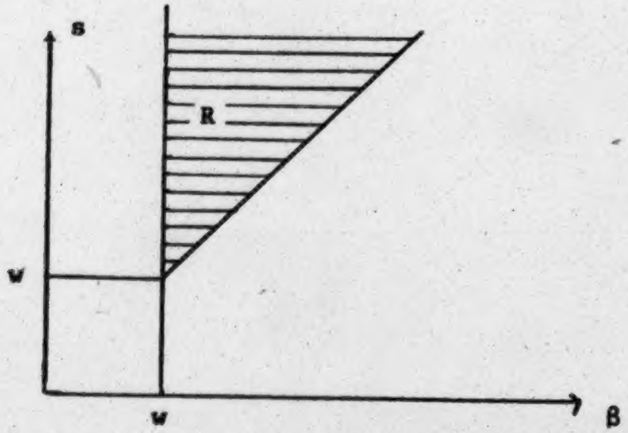

Figure 9

Plane Integration

The function $\dfrac{h(s)}{\sqrt{\beta-w}\,\sqrt{s-\beta}}$ is to be integrated over the region R shown on the previous page. One can cover this same region by performing the β integration first. We get

$$\int_w^\infty \frac{g(\beta)\ d\beta}{\sqrt{\beta-w}} = \int_{s=w}^\infty \left(h(s) \int_{\beta=w}^{s} \frac{d\beta}{\sqrt{(\beta-w)(s-\beta)}} \right) ds \quad .$$

Observe that $\displaystyle\int_{\beta=w}^{s} \frac{d\beta}{\sqrt{(\beta-w)(s-\beta)}} = \int_{-1}^{1} \frac{du}{\sqrt{1-u^2}} = \pi$. Also $g(\beta) = 0$ and $h(s) = 0$ for all sufficiently large β and s . Thus we have

$$\int_w^\infty \frac{g(\beta)\ d\beta}{\sqrt{\beta-w}} = \pi \int_{s=w}^\infty h(s)\ ds \quad .$$

This means $h(w) = -\dfrac{1}{\pi}\dfrac{\partial}{\partial w}\left[\displaystyle\int_w^\infty \frac{g(\beta)\ d\beta}{\sqrt{\beta-w}}\right]$. Substitute $g(\beta) = \partial_t(\beta^{1/2}, v_0)$ and set $w = s$ and $h(w) = h(s) = \dfrac{\gamma(s^{1/2})}{v_0\ s^{1/2}}$ to get

$$\gamma(s^{1/2}) = -v_0\ \frac{s^{1/2}}{\pi}\ \frac{\partial}{\partial s}\left[\int_s^\infty \frac{\partial_t(\beta^{1/2}, v_0) d\beta}{\sqrt{\beta-s}}\right] \quad .$$

We now make the transformations $u^2 = s$ and $\beta = b^2$ to obtain

$$\gamma(u) = -\frac{v_0}{\pi}\ \frac{\partial}{\partial u}\left[\int_u^\infty \frac{\partial_t(b, v_0) b\ db}{\sqrt{b^2 - u^2}}\right] \quad . \tag{9}$$

Recall that $\gamma(u) + u = a^{-1}(u) a^{-1'}(u) = \dfrac{1}{2}\dfrac{d}{du}\left([a^{-1}(u)]^2\right)$. This can be explicitly integrated. The result is

$$-\frac{v_0}{\pi}\int_u^\infty \frac{\partial_t(b,v_0)b\,db}{\sqrt{b^2-u^2}} + \frac{u^2}{2} = \frac{[a^{-1}(u)]^2}{2} + \text{constant.}$$

For $u > A$, $a^{-1}(u) = u$ and the time delay is zero (no interation). This shows us that the constant of integration is zero and hence

$$[a^{-1}(u)]^2 - u^2 = -2\frac{v_0}{\pi}\int_u^\infty \frac{\partial_t(b,v_0)b\,db}{\sqrt{b^2-u^2}} \geq 0$$

for a positive potential since $a(r) \leq r$ and so $a^{-1}(u) \geq u > 0$. This means $\partial_t(b,v_0)$ is negative in general and we have a time advance rather than a time delay. This is not surprizing since the free particle path is longer than the actual path.

We can determine the function $a^{-1}(u)$ from the time delay ∂_t and we know $a(r) = r\sqrt{1 - \frac{2}{m v_0^2}V(r)}$. Hence by measuring ∂_t as a function of b for a given fixed v_0 we can determine $V(r)$. The fundamental results are

$$[a^{-1}(u)]^2 = u^2 - 2\frac{v_0}{\pi}\int_u^\infty \frac{\partial_t(b,v_0)b\,db}{\sqrt{b^2-u^2}}, \tag{10}$$

$$a(r) = r\sqrt{1 - \frac{2}{m v_0^2}V(r)}.$$

The potential $V(r)$ must be such that $a(r)$ is monotone increasing in r, invertible, with differentiable inverse. If v_0 and r are sufficiently large, this is true.

Impact Parameter - Scattering Intensities

Suppose we have a uniform beam of particles incident upon a scattering central potential. Suppose furthermore, the beam has intensity I_0 particles per unit area per unit time when directed on an area orthogonal to the beam. Suppose $I_s(\theta)$ particles per unit solid angle per unit time are detected at a scattering angle θ from the initial direction. Then the differential scattering cross section is $\frac{d\sigma}{d\Omega} = \frac{I_s(\theta)}{I_0}$, where $d\sigma$ is a unit of area at a specified location in the incident beam, such that all particles passing through $d\sigma$ pass through the specified element of solid angle $d\Omega$ located at the scattering angle θ. Because of radial dependence in the potential, we have no ϕ dependence in scattering. $\frac{d\sigma}{d\Omega}$ as a function of θ can be measured experimentally from $\frac{I_s(\theta)}{I_0}$. Alternatively, this can be used to relate the impact parameter to the scattering angle, and gives us a means to get $\theta_s(b)$ for fixed v_0. We have

$$d\sigma = b\,db\,d\phi = b\left|\frac{db}{d(-\cos\theta)}\right| d(-\cos\theta)\,d\phi$$

$$= b\left|\frac{db}{d(-\cos\theta)}\right| d\Omega = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right| d\Omega \quad .$$

Hence $-\left[\frac{d\sigma}{d\Omega}\right](\theta)\sin\theta\,d\theta = b\,db$ for negative $\frac{db}{d\theta}$ and so for total reflection at π, $b^2 = \frac{2}{I_0}\int_{\theta_s}^{\pi} I_s(\theta)\sin\theta\,d\theta$.

In general ∂_t is known as a function of v_0 and θ_s rather than v_0 and b. However with this additional information, ∂_t can be obtained as a function of b, and thus the results in (10) can be applied.

Total Reflection or Transmission

Let us consider $\partial_t(b,v_0)$ where $b = 0$ as a function of v_0. In this case we return to the problem in one dimension. Either the particle is reflected back along its initial path $\theta_s = \pi$, or it overcomes the potential and passes through $\theta_s = 0$. In either case $\partial_t(0,v_0)$ can be measured as a function of v_0 and this provides information about the potential. Substituting $b = 0$ in an earlier expression for ∂t we get

$$\partial t = \frac{2}{v_0}\int_{r_{min}}^{A} \frac{r\,dr}{\sqrt{[a(r)]^2 - b^2}} - \frac{2}{v_0}\int_{b}^{A} \frac{r\,dr}{\sqrt{r^2 - b^2}}$$

$$= \frac{2}{v_0}\int_{r_{min}}^{A} \frac{dr}{\sqrt{1 - \frac{2}{mv_0^2}V(r)}} - \frac{2A}{v_0} \quad .$$

If $r_{min} > 0$ one has reflection, while if $r_{min} = 0$ one has transmission, At any case, for $r_{min} > 0$, $V(r_{min}) = \frac{1}{2} m v_0^2$ and for $r_{min} = 0$, $V(r_{min}) \leq \frac{1}{2} m v_0^2$.

The case of transmission has already been dealt with in one dimensional problems. Let us assume reflection $(r_{min} > 0)$. Let us also suppose $V(r)$ is a monotone decreasing positive function of positive r which is zero for $r \geq A$. We have

$$\partial t(0,v_0) + \frac{2A}{v_0} = 2\int_{r_{min}}^{A} \frac{dr}{\sqrt{v_0^2 - \frac{2}{m}V(r)}} \; , \quad r_{min} = V^{-1}\left(\frac{mv_0^2}{2}\right) \quad .$$

We change the variable of integration in this last integral.

$$\partial t(0,v_0) + \frac{2A}{v_0} = 2\int_{v_0^2}^{2/m\,V(A)} \frac{V^{-1'}(\frac{mu}{2})\,\frac{m}{2}\,du}{\sqrt{v_0^2 - u}}$$

$$= -m\int_0^{v_0^2} \frac{V^{-1'}(\frac{mu}{2})\,du}{\sqrt{v_0^2 - u}} \quad .$$

For this to hold A must be a very special point uniquely determined from the potential. We require $V(r) \equiv 0$ for $r > A$ and $V(r) > 0$ for $r < A$ and $V(r)$ strictly monotone decreasing for $0 < r < A$. Let $v_0^2 = \beta$, $g(\beta) = \partial t(0,\beta^{1/2}) + \frac{2A}{\beta^{1/2}}$ and $h(u) = -m\,V^{-1'}(\frac{mu}{2})$. Then $g(\beta) = \int_0^\beta \frac{h(u)\,du}{\sqrt{\beta-u}}$. This can be inverted (details omitted) to get $h(u) = \frac{1}{\pi}\frac{\partial}{\partial u}\left[\int_0^u \frac{g(\beta)\,d\beta}{\sqrt{u-\beta}}\right]$. By substituting back we eventually get (' refers to $\frac{d}{dE} = \frac{2}{m}\frac{d}{du}$)

$$-m\,V^{-1'}(\frac{mu}{2}) = \frac{1}{\pi}\frac{\partial}{\partial u}\left[\int_{0,}^{u^{1/2}} \frac{[\partial_t(0,v_0) + \frac{2A}{v_0}]\,2v_0\,d\,v_0}{\sqrt{u - v_0^2}}\right] \quad .$$

This solution is complete except for one difficulty. The range A of the potential must be known in order to complete the potential $V(r)$. This same problem appeared in one dimensional classical time delay in scattering. The integral involving A can be separated out and directly integrated. However first we can integrate the entire equation over u to get

$$V^{-1}(\frac{mu}{2}) = -\frac{1}{2\pi}\int_0^{u^{1/2}} \frac{[\partial_t(0,v_0) + \frac{2A}{v_0}]\, 2v_0\, d\, v_0}{\sqrt{u - v_0^2}} + A ,$$

the constant of integration determined to be A from the condition $u = 0$. Now integrating the coefficient of A we get cancellation of A and

$$V^{-1}(\frac{mu}{2}) = -\frac{1}{2\pi}\int_0^{u^{1/2}} \frac{\partial_t(0,v_0)\, 2v_0\, dv_0}{\sqrt{u - v_0^2}} , \quad \text{or}$$

$$V^{-1}(\frac{mu}{2}) = -\frac{1}{\pi}\int_0^{u^{1/2}} \frac{\partial_t(0,v_0)\, v_0\, d\, v_0}{\sqrt{u - v_0^2}} . \qquad (11)$$

Notice that A has cancelled out of the expression and so the difficulty of knowing the point at which the potential vanishes has disappeared. (11) can be treated as a general result for monotone decreasing $V(r)$ that approach zero. Equations (10) and (11) also indicate the importance of the impact parameter time delay ∂_t and the ease of inversion.

Example of Time Delay and Potential

Let us take the potential $V(r)$ to be $V(r) = \frac{mv_1^2(c^2-r^2)}{2r^2}$ for $0 < r < c$ and $V(r) = 0$ for $r > c$. We recall $a(r) = r\sqrt{1 - \frac{2}{mv_0^2}V(r)}$ so that substitution gives $a(r) = \sqrt{[1 + \frac{v_1^2}{v_0^2}]\, r^2 - (\frac{v_1}{v_0}c)^2}$ for $a^{-1}(0) \leq r \leq c$. Inverting we get $a^{-1}(u) = \sqrt{u^2 + (\frac{v_1}{v_0}c)^2} \Big/ \sqrt{1 + \frac{v_1^2}{v_0^2}}$.

Hence (for $c \geq u \geq 0$)

$$[a^{-1}(u)]^2 - u^2 = \frac{v_1^2(c^2-u^2)}{v_0^2 + v_1^2} = -2\,\frac{v_0}{\pi}\int_u^\infty \frac{\partial t(b,v_0)b\,db}{\sqrt{b^2 - u^2}}$$

by (10). Consequently $\partial t(b,v_0)$ must satisfy

$$\frac{v_1^2(c^2-u^2)}{v_0^2 + v_1^2} = -\,\frac{2v_0}{\pi}\int_u^\infty \frac{\partial t(b,v_0)b\,db}{\sqrt{b^2 - u^2}}$$

for $c > u > 0$.

Now let us determine $\partial t(b,v_0)$. First of all $\partial t(b,v_0) = 0$ for $b > c$ since the potential $V(r)$ has range c and consequently any greater impact parameter than c misses the potential. So let us suppose $b < c$. We have

$$\partial t(b,v_0) = \frac{2}{v_0}\int_{r_{min}}^{c} \frac{r\,dr}{\sqrt{[a(r)]^2 - b^2}} - \frac{2}{v_0}\int_b^c \frac{r\,dr}{\sqrt{r^2 - b^2}} \; ,$$

where $r_{min} = a^{-1}(b) = \sqrt{b^2 + (\frac{v_1}{v_0}\,c)^2} \Big/ \sqrt{1 + \frac{v_1^2}{v_0^2}} < c$ for $b < c$. Observe that $\sqrt{[a(r)]^2 - b^2} = \sqrt{1 + \frac{v_1^2}{v_0^2}}\,\sqrt{r^2 - r_{min}^2}$. Thus

$$\partial t(b,v_0) = \frac{2}{v_0\sqrt{1 + v_1^2/v_0^2}}\int_{r_{min}}^{c} \frac{r\,dr}{\sqrt{r^2 - r_{min}^2}} - \frac{2}{v_0}\int_b^c \frac{r\,dr}{\sqrt{r^2 - b^2}}$$

$$= \frac{2}{v_0\sqrt{1 + v_1^2/v_0^2}}\,\sqrt{c^2 - r_{min}^2} - \frac{2}{v_0}\sqrt{c^2 - b^2}$$

$$= -\frac{2\sqrt{c^2-b^2}}{v_0}\left(\frac{v_1^2}{v_0^2+v_1^2}\right) .$$

Thus we obtain the explicit time delay (which is negative, meaning a time advance) for this example as

$$\partial t = -\frac{2\sqrt{c^2-b^2}}{v_0}\left(\frac{v_1^2}{v_0^2+v_1^2}\right) = \partial t(b,v_0) .$$

Note that v_1 and c are parameters determined by the potential, and are part of the definition of $V(r)$. Now consider substituting this into the integral of time delay above, namely

$$-\frac{2v_0}{\pi}\int_u^\infty \frac{\partial t(b,v_0)b\ db}{\sqrt{b^2-u^2}} = -\frac{2v_0}{\pi}\int_u^c \frac{\partial t(b,v_0)b\ db}{\sqrt{b^2-u^2}}$$

for $c \geq u \geq 0$, since $\partial t(b,v_0) = 0$ for $b > c$. Thus our integral becomes

$$\frac{4}{\pi}\left(\frac{v_1^2}{v_0^2+v_1^2}\right)\int_u^c \frac{\sqrt{c^2-b^2}\ b\ db}{\sqrt{b^2-u^2}} = \frac{4}{\pi}\left(\frac{v_1^2}{v_0^2+v_1^2}\right)\int_0^w \sqrt{w^2-\lambda^2}\ d\lambda$$

where $\lambda = \sqrt{b^2-u^2}$ and $w = \sqrt{c^2-u^2}$. Integrating we get $\frac{4}{\pi}\left(\frac{v_1^2}{v_0^2+v_1^2}\right) w^2\frac{\pi}{4} = \left(\frac{v_1^2}{v_0^2+v_1^2}\right)(c^2-u^2)$. This proves that

$$\frac{v_1^2(c^2-u^2)}{v_0^2+v_1^2} = -\frac{2v_0}{\pi}\int_u^\infty \frac{\partial t(b,v_0)b\ db}{\sqrt{b^2-u^2}}$$

in agreement with equations (10).

At the same time let us test the validity of equation (11) on this example. Using $\partial t(b,v_0)$ above, we can set $b = 0$ to get $\partial t(0,v_0) = -\frac{2c}{v_0}\left(\frac{v_1^2}{v_0^2 + v_1^2}\right)$. Substitute this into the integral of equation (11) to get

$$-\frac{1}{\pi}\int_0^{u^{1/2}} \frac{\partial_t(0,v_0)v_0\,dv_0}{\sqrt{u - v_0^2}} = \frac{2cv_1^2}{\pi}\int_0^{u^{1/2}} \frac{d\,v_0}{(v_0^2 + v_1^2)\sqrt{u - v_0^2}} .$$

In this last integral make the substitution $w = v_1\sqrt{\frac{u}{v_0^2} - 1} \,/\, \sqrt{u + v_1^2}$ in place of v_0 and get $\frac{2c\,v_1}{\pi\sqrt{u + v_1^2}}\int_0^\infty \frac{dw}{1 + w^2} = \frac{v_1 c}{\sqrt{u + v_1^2}}$. According to equation (11) we have $V^{-1}(\frac{mu}{2}) = r = \frac{v_1 c}{\sqrt{u + v_1^2}}$ for $u > 0$. If we invert and solve for $V(r)$ we get $V(r) = \frac{mu}{2} = \frac{mv_1^2}{2r^2}(c^2 - r^2)$ for $r < c$.

The Scattering Angle and Its Inversion

The objective in this section is to determine the potential $V(r)$ given the scattering angle θ_s as a function of b , the impact parameter. As we have seen, this function can be obtained by experimental measurement since $b^2 = \frac{2}{I_0}\int_{\theta_s}^{\pi} I_s(\theta)\sin\theta\,d\theta$. Also

$$\theta_s(b) = \pi - 2b\, v_0 \int_{r_{\min}}^{\infty} \frac{dr}{r^2\sqrt{v_0^2[1 - \frac{b^2}{r^2}] - \frac{2}{M} V(r)}} .$$

We assume that the particles all have the same mass in the beam being scattered, and all the same (vector) velocity with magnitude v_0 . Define $a(r) = r\sqrt{1 - \frac{2}{m v_0^2} V(r)}$. Then $\theta_s(b) = \pi - 2b \int_{r_{\min}}^{\infty} \frac{dr}{r\sqrt{[a(r)]^2 - b^2}}$ where $r_{\min} = a^{-1}(b)$. Since $\pi = 2b \int_b^{\infty} \frac{dr}{r\sqrt{r^2 - b^2}}$ we have

$$\frac{\theta_s(b)}{2b} = \int_b^{\infty} \frac{dr}{r\sqrt{r^2 - b^2}} - \int_{a^{-1}(b)}^{\infty} \frac{dr}{r\sqrt{[a(r)]^2 - b^2}} .$$

We make the transformation $r = c\, e^{\lambda}$ and $f(\lambda) = a(ce^{\lambda})$ to get

$$\frac{\theta_s(b)}{2b} = \int_{\log(\frac{b}{c})}^{\infty} \frac{d\lambda}{\sqrt{c^2 e^{2\lambda} - b^2}} - \int_{f^{-1}(b)}^{\infty} \frac{d\lambda}{\sqrt{[f(\lambda)]^2 - b^2}} .$$

We substitute $s = f(\lambda)$ in the second integral and $r = ce^{\lambda}$ in the first integral to get

$$\frac{\theta_s(b)}{2b} = \int_b^{\infty} \frac{\frac{1}{r}\, dr}{\sqrt{r^2 - b^2}} - \int_b^{\infty} \frac{f^{-1\prime}(s)\, ds}{\sqrt{s^2 - b^2}}$$

$$= \int_b^{\infty} \frac{[\frac{1}{r} - f^{-1\prime}(r)]\, dr}{\sqrt{r^2 - b^2}} = \int_b^{\infty} \frac{\gamma(r)\, dr}{\sqrt{r^2 - b^2}} .$$

where $\gamma(r) = \frac{1}{r} - f^{-1'}(r)$. In the equation $\frac{\theta_s(b)}{2b} = \int_b^\infty \frac{\gamma(r)\,dr}{\sqrt{r^2 - b^2}}$

substitute $\beta = b^2$ and $\sigma = r^2$ to get $\frac{\theta_s(\beta^{1/2})}{2\,\beta^{1/2}} = \int_\beta^\infty \frac{\gamma(\sigma^{1/2})\,\frac{1}{2}\,\sigma^{-1/2}\,d\sigma}{\sqrt{\sigma - \beta}}$.

This is of the form $g(\beta) = \int_\beta^\infty \frac{h(\sigma)\,d\sigma}{\sqrt{\sigma-\beta}}$ with inverse
$h(\sigma) = -\frac{1}{\pi}\frac{d}{d\sigma}\left[\int_\sigma^\infty \frac{g(\beta)\,d\beta}{\sqrt{\beta-\sigma}}\right]$. Also note that $g(\beta) = \frac{\theta_s(\beta^{1/2})}{\beta^{1/2}}$ and

$h(\sigma) = \gamma(\sigma^{1/2})\sigma^{-1/2}$. Thus $\gamma(\sigma^{1/2})\sigma^{-1/2} = -\frac{1}{\pi}\frac{d}{d\sigma}\left[\int_\sigma^\infty \frac{\theta_s(\beta^{1/2})\beta^{-1/2}\,d\beta}{\sqrt{\beta-\sigma}}\right]$.

We switch back using $\beta = b^2$ and $\sigma = r^2$ to get

$$\gamma(r) = -\frac{1}{\pi}\frac{d}{dr}\left[\int_r^\infty \frac{\theta_s(b)\,db}{\sqrt{b^2 - r^2}}\right] .$$

Writing $\gamma(r)$ as $\frac{1}{r} - f^{-1'}(r)$ we can integrate over r to get

$$\log\left(\frac{r}{c}\right) - f^{-1}(r) = -\frac{1}{\pi}\int_r^\infty \frac{\theta_s(b)\,db}{\sqrt{b^2 - r^2}} .$$

The constant of integration is zero since $f^{-1}(r) = \log\left(\frac{r}{c}\right)$ for $r > A$ the range of the potential. We also know that $\theta_s(b) = 0$ if $b > A$. Observe that we can calculate $f^{-1}(s)$. If $f^{-1}(s) = \lambda$ then $s = f(\lambda) = a(ce^\lambda)$. Thus $ce^\lambda = a^{-1}(s)$ and $\lambda = \log\left(\frac{a^{-1}(s)}{c}\right) = f^{-1}(s)$. If we substitute $f^{-1}(r) = \log\left(\frac{a^{-1}(r)}{c}\right)$ in the above expression we get

$$\log\left(\frac{a^{-1}(s)}{s}\right) = \frac{1}{\pi}\int_s^\infty \frac{\theta_s(b)\,db}{\sqrt{b^2 - s^2}} \quad .$$

Hence

$$a^{-1}(s) = s \exp\left(\frac{1}{\pi}\int_s^\infty \frac{\theta_s(b)\,db}{\sqrt{b^2 - s^2}}\right) \quad ,$$

$$a(r) = r\sqrt{1 - \frac{2}{mv_0^2}V(r)} \quad . \qquad (12)$$

Example 1. Suppose we are given that the scattering angle $\theta_s(b)$ for fixed v_0 behaves like $\theta_s = 2 \arctan\left(\frac{e^2}{v_0^2\, bm}\right)$. Use equations (12) to solve for the potential $V(r)$.

First of all, we obtain $a^{-1}(s)$ given by

$$a^{-1}(s) = s \exp\left(\frac{1}{\pi}\int_s^\infty \frac{2 \arctan\left(\frac{e^2}{v_0^2\, mb}\right) db}{\sqrt{b^2 - s^2}}\right) .$$

For economy of notation we can let $c = \frac{e^2}{v_0^2\, m}$ and so $\theta_s = 2 \arctan\left(\frac{c}{b}\right)$ and $a^{-1}(s) = s \exp\left(\frac{1}{\pi}\int_s^\infty \frac{2 \arctan\left(\frac{c}{b}\right) db}{\sqrt{b^2 - s^2}}\right)$. Let us examine $\int_s^\infty \frac{2 \arctan\left(\frac{c}{b}\right) db}{\sqrt{b^2 - s^2}}$ and attempt to get is value. If we look at its derivative with respect to c we have

$$\frac{\partial}{\partial c}\int_s^\infty \frac{2\arctan\left(\frac{c}{b}\right)db}{\sqrt{b^2-s^2}} = \int_s^\infty \frac{2\,db}{(b^2+c^2)\sqrt{1-s^2/b^2}}$$

$$= \int_{s^2}^\infty \frac{d\beta}{(\beta+c^2)\sqrt{\beta-s^2}} \quad \text{for} \quad \beta = b^2 \quad .$$

Now transform this last integral with $\sqrt{\beta-s^2} = \sqrt{s^2+c^2}\tan\phi$ and integrate over ϕ instead of β. The result of integration is $\pi/\sqrt{s^2+c^2}$. A function with this as a derivative with respect to c is $\pi\sinh^{-1}\left(\frac{c}{s}\right)$, and so

$$\int_s^\infty \frac{2\arctan\left(\frac{c}{b}\right)db}{\sqrt{b^2-s^2}} = \pi\sinh^{-1}\left(\frac{c}{s}\right) \quad .$$

Since both sides are zero for $c = 0$ we have no integration constant. Using an alternative form for $\sinh^{-1}\left(\frac{c}{s}\right)$ we have

$$\int_s^\infty \frac{2\arctan\left(\frac{c}{b}\right)db}{\sqrt{b^2-s^2}} = \pi\log\left(\frac{c}{s}+\frac{1}{s}\sqrt{c^2+s^2}\right) \quad .$$

This means we can obtain $a^{-1}(s)$ as

$$a^{-1}(s) = s\exp\frac{1}{\pi}\int_s^\infty \frac{2\arctan\left(\frac{c}{b}\right)db}{\sqrt{b^2-s^2}} = c+\sqrt{c^2+s^2} \quad .$$

$$a^{-1}(s) = r = c+\sqrt{c^2+s^2} \quad .$$

We can solve $s = a(r)$ and get $s = \sqrt{r^2-2rc} = a(r) = r\sqrt{1-\frac{2c}{r}} = r\sqrt{1-\left(2/mv_0^2\right)V(r)}$. This means that $V(r) = mv_0^2c/r = e^2/r$. This proves that the unique potential with the given scattering angle $\theta_s(b)$ as $\theta_s(b) = 2 \arctan\left(\frac{e^2}{v_0^2 bm}\right)$ is the Coulomb potential $V(r) = \frac{e^2}{r}$.

Example 2. Suppose $\frac{d\sigma}{d\Omega}$ is measured experimentally and found to be equal to $\frac{e^4}{4\, v_0^4\, m^2 \sin^4\left(\frac{\theta}{2}\right)}$. What is $\theta_s(b)$? Recall that $b^2 = 2 \int_{\theta_s}^{\pi} \frac{d\sigma}{d\Omega}(\theta) \sin\theta \, d\theta$, and so we substitute to get

$$b^2 = 2 \int_{\theta_s}^{\pi} \frac{e^4}{4\, v_0^4\, m^2 \sin^4\left(\frac{\theta}{2}\right)} 2 \sin\frac{\theta}{2} \cos\frac{\theta}{2} \, d\theta \quad ,$$

$$= \frac{e^4}{v_0^4\, m^2} \cot^2 \frac{\theta_s}{2} \quad .$$

Thus $b = \frac{e^2}{v_0^2\, m} \cot\frac{\theta_s}{2}$ and so $\tan\frac{\theta_s}{2} = \frac{e^2}{b\, v_0^2\, m}$ and $\theta_s = 2 \arctan\left(\frac{e^2}{b v_0^2\, m}\right)$ gives θ_s as a function of b for fixed v_0. In view of the above results, we see that the potential which produces this scattering data must be $V(r) = \frac{e^2}{r}$.

CHAPTER IV

TIME OF ARRIVAL IN CLASSICAL MECHANICS

Consider the one dimensional Hamiltonian with the properties, $H(p,q) = \frac{p^2}{2M} + V(q)$, $\frac{\partial H}{\partial p} = \dot{q}$, $\frac{\partial H}{\partial q} = -\dot{p}$. We select functions $\tau(p,q)$ and $\tau_0(p,q,t)$ such that $\{H,\tau\} = 1$, $\tau_0 = t + \tau$,

$$\frac{d\tau_0}{dt} = 1 + [\frac{\partial\tau}{\partial q}\dot{q} + \frac{\partial\tau}{\partial p}\dot{p}] = 1 + \frac{\partial\tau}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial\tau}{\partial p}\frac{\partial H}{\partial q} = 0 \quad ,$$

$$\{H,\tau\} = \frac{\partial H}{\partial q}\frac{\partial\tau}{\partial p} - \frac{\partial H}{\partial p}\frac{\partial\tau}{\partial q} = 1 \quad .$$

Like H , τ_0 is a constant of the motion. Consider linear motion in one dimension $p = M\dot{q}$, $H - V(q) = \frac{p^2}{2M} = \frac{1}{2}M\dot{q}^2$.

We see that the equation $\{H,\tau\} = 1$ determines τ uniquely up to an additive function τ_1 of p and q which is a constant of motion for this Hamiltonian. We observe

$$\{H,\tau_1\} = 0 \leftrightarrow \frac{d\tau_1}{dt} = 0 \quad \text{if} \quad \tau_1 = \tau_1(p,q) \; .$$

This is true if and only if $\frac{\partial H}{\partial q}\frac{\partial\tau_1}{\partial p} = \frac{\partial H}{\partial p}\frac{\partial\tau_1}{\partial q}$ where $\frac{\partial H}{\partial q} = V'(q)$ and $\frac{\partial H}{\partial p} = \frac{p}{M} = \dot{q}$. We can solve for τ_1 . Observe that $V'(q)\frac{\partial\tau_1}{\partial p} = \frac{p}{M}\frac{\partial\tau_1}{\partial q}$. This characterizes a constant τ_1 of the motion. From this we get

$\frac{\partial\tau_1}{\partial q} = \frac{MV'(q)}{p}\frac{\partial\tau_1}{\partial p}$. Let $\frac{\partial\tau_1}{\partial p} = pf(q,p)$. Then $\frac{\partial\tau_1}{\partial q} = MV'(q)\, f(q,p)$ and $\frac{\partial^2\tau_1}{\partial q\partial p} = MV'(q)\frac{\partial f}{\partial p} = p\frac{\partial f}{\partial q}$. Hence f is also a constant of motion, since it satisfies the same equation as τ_1 . Observe $f(q,p) = \frac{1}{p}\frac{\partial\tau_1}{\partial p}$. Any function g of the Hamiltonian, i.e., $g(H(q,p))$ is a constant of motion.

Now let us solve $\{H,\tau\} = 1$. One solution $\tau(p,q)$ of this equation is $\tau = -\sqrt{\frac{M}{2}}\int_{q_0}^{q}\frac{dx}{\sqrt{p^2/2M + V(q) - V(x)}}$ for arbitrary q_0 . In general we have

$$\tau(p,q) = \tau = -\sqrt{\frac{M}{2}}\int_{q_0}^{q}\frac{dx}{\sqrt{p^2/2M + V(q) - V(x)}} + g\left(\frac{p^2}{2M} + V(q)\right) ,$$

for some function g . q_0 is a constant independent of p,q or t . Changing the value of q_0 affects the function g if τ is maintained. We have the function τ_0 of p,q and t given by $\tau_0 = t + \tau$ where τ is defined above. τ_0 is a constant of the motion.

This solves the one dimensional case. Let us try the same type of calculations for the radial potential in three dimensions, namely $H = \frac{p_r^2}{2M} + \frac{L^2}{2Mr^2} + V(r)$.

The coordinates are r,θ where $L = mr^2\dot{\theta} = p_\theta$ is constant. The momenta are p_r, L where $p_r = m\dot{r}$.

We have the equations of motion given by $\frac{\partial H}{\partial p_\theta} = \dot{\theta}$, $\frac{\partial H}{\partial p_r} = \dot{r}$,

$\frac{\partial H}{\partial \theta} = -\dot{p}_\theta = 0$, $\frac{\partial H}{\partial r} = -\dot{p}_r$ where $H = \frac{p_r^2}{2M} + \frac{p_\theta^2}{2Mr^2} + V(r) = H(\underbrace{p_r,p_\theta}_{p},\underbrace{r,\theta}_{q})$

is independent of θ .

Consider $\tau_0 = t + \tau$ a constant of the motion, where τ is a function of p_r , p_θ , r , θ so that $\{H,\tau\} = \frac{\partial H}{\partial r}\frac{\partial \tau}{\partial p_r} + \frac{\partial H}{\partial \theta}\frac{\partial \tau}{\partial p_\theta} - \frac{\partial H}{\partial p_r}\frac{\partial \tau}{\partial r} - \frac{\partial H}{\partial p_\theta}\frac{\partial \tau}{\partial \theta} = 1$. Substituting for $\frac{\partial H}{\partial r}$, $\frac{\partial H}{\partial p_r}$, and $\frac{\partial H}{\partial p_\theta}$ we get

$$1 = [V'(r) - \frac{p_\theta^2}{Mr^3}]\frac{\partial \tau}{\partial p_r} - \frac{p_r}{M}\frac{\partial \tau}{\partial r} - \frac{p_\theta}{Mr^2}\frac{\partial \tau}{\partial \theta} .$$

As in the one dimensional case, the equation $\{H,\tau\} = 1$ determines τ uniquely up to an additive function $\tau_1(p_r,p_\theta,r,\theta)$ which satisfies $\{H,\tau_1\} = 0$, i.e. $\frac{d\tau_1}{dt} = 0$, so τ_1 is a constant of the motion. The most general constant of the motion, which is a function of p_r,p_θ,r,θ only (as is τ_1) is $g(H,p_\theta)$. Hence we may simply determine any solution τ to $\{H,\tau\} = 1$ and add $g(\frac{p_r^2}{2M} + \frac{p_\theta^2}{2Mr^2} + V(r),p_\theta)$. One such solution is

$$\tau = -\sqrt{\frac{M}{2}}\int_{r_0}^{r} \frac{ds}{\sqrt{(\frac{p_r^2}{2M} + \frac{p_\theta^2}{2Mr^2} + V(r)) - (\frac{p_\theta^2}{2Ms^2} + V(s))}}$$

to the equation $\{H,\tau\} = 1$ which as we saw, can be written as

$$1 = [V'(r) - \frac{p_\theta^2}{Mr^3}]\frac{\partial \tau}{\partial p_r} - \frac{p_r}{M}\frac{\partial \tau}{\partial r} - \frac{p_\theta}{Mr^2}\frac{\partial \tau}{\partial \theta} .$$

Hence the most general solution is

$$\tau = -\sqrt{\frac{M}{2}}\int_{r_0}^{r} \frac{ds}{\sqrt{p_r^2/2M + p_\theta^2/2Mr^2 + V(r) - p_\theta^2/2Ms^2 - V(s)}}$$

$$+ g\left(\frac{p_r^2}{2M} + \frac{p_\theta^2}{2Mr^2} + V(r)\ ,\ p_\theta\right)$$

, where $\tau = \tau(p_r, p_\theta, r, \theta)$ is independent of θ. If r_0 is varied g must be varied in order to maintain τ, and this is possible as one can easily see. Also $\tau_0 = t + \tau$ will be a constant of the motion for any one of the above values of τ.

CHAPTER V

SCATTERING THEORY AND THE TIME OPERATOR

Consider the Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} \psi = H\psi = (H_1+H_2)\psi \quad .$$

Example: $H_1 = -\frac{h^2}{2m} \nabla^2$, kinetic energy,

$H_2 = V(\vec{r})$, potential function (assumed short range).

We assume a continuous energy distribution. Let $\psi_\omega(\vec{r})$ denote energy eigenfunctions satisfying $H\psi_\omega(\vec{r}) = \hbar\omega\psi_\omega(\vec{r})$. Then $\psi_\omega(\vec{r})\, e^{-i\omega t}$ solves the equation $i\hbar \frac{\partial\psi}{\partial t} = H\psi$. We may superimpose solutions as

$$\psi(\vec{r},t) = \int_0^\infty A(\omega)\, \psi_\omega(\vec{r})\, e^{-i\omega t}\, d\omega \quad . \tag{1}$$

The solution $\psi_\omega(\vec{r})$ to $H\psi_\omega(\vec{r}) = \hbar\omega\psi_\omega(r)$ need not be unique. We do require that for each ω , one particular solution $\psi_\omega(\vec{r})$ is selected so that

$$\int_{\substack{\text{all}\\\text{space}}} \psi^*_{\omega_1}(\vec{r})\, \psi_{\omega_2}(\vec{r})\, d\vec{r} = \delta(\omega_1-\omega_2) \quad , \tag{2}$$

for the representation of the particular wavefunction $\Psi(r,t)$. We assume that any $\psi(\vec{r},t)$ can be represented this way.

Normalization

We insist that $\int_{\substack{\text{all}\\ \text{space}}} |\psi(\vec{r},t)|^2 \, d\vec{r} = 1$ for all t . Then .

$$\psi(\vec{r},t) = \int_0^\infty A(\omega)\, \psi_\omega(\vec{r})\, e^{-i\omega t}\, d\omega \quad , \text{ and } \quad \psi^*(\vec{r},t) = \int_0^\infty A^*(\omega')\psi^*_{\omega'}(\vec{r})\, e^{+i\omega' t} d\omega' ,$$

so

$$\int_{\substack{\text{all}\\ \text{space}}} |\psi(\vec{r},t)|^2 d\vec{r} = \int_0^\infty \int_0^\infty A^*(\omega')A(\omega)\, e^{i(\omega'-\omega)t}\, d\omega d\omega'\, \delta(\omega-\omega')$$

$$= \int_0^\infty |A(\omega)|^2 \, d\omega = 1 \quad .$$

Let us evaluate the expectation value of the Hamiltonian H .

$$\langle H\rangle_t = \int_{\substack{\text{all}\\ \text{space}}} \psi^*(\vec{r},t)\, H\psi(\vec{r},t)\, d\vec{r}$$

$$= \int_0^\infty \int_0^\infty A^*(\omega')A(\omega)\, e^{i(\omega'-\omega)t}\, d\omega d\omega'\, \hbar\omega\, \delta(\omega-\omega')$$

$$= \int_0^\infty A^*(\omega)\, \hbar\omega\, A(\omega)\, d\omega \quad .$$

The expectation value of $\hbar\omega$ with respect to $A(\omega)$ is $\langle H\rangle$. Now consider

$$\psi(\vec{r},t) = \int_0^\infty A(\omega)\, \psi_\omega(\vec{r})\, e^{-i\omega t}\, d\omega \quad .$$

Multiply by $\psi^*_{\omega'}(\vec{r})$ and integrate over all space. The eventual result is

$$A(\omega) = e^{i\omega t_0} \int_{\text{space}} \psi^*_\omega(\vec{r}\,')\psi(\vec{r}\,',t_0)\, d\vec{r}\,' \quad , \tag{3}$$

for any t_0. The right hand side above is independent of t_0. Substituting, we get $\psi(\vec{r},t) = \int_{\text{space}} T_{(t-t_0)}(\vec{r},\vec{r}\,')d\vec{r}\,'\ \psi(\vec{r}\,',t_0)$ where

$$T_{(t-t_0)}(\vec{r},\vec{r}\,') = \int_0^\infty \psi^*_\omega(\vec{r}\,')\ \psi_\omega(\vec{r})\ e^{-i\omega(t-t_0)}\, d\omega \tag{4}$$

is the time shift operator for the position wave function, only for wave functions derived from expansions in the particular energy eigenfunctions $\psi_\omega(\vec{r})$.

Phase Uncertaininity in $A(\omega)$

For given $\psi(\vec{r},t) = \int_0^\infty A(\omega)\ \psi_\omega(\vec{r})\ e^{-i\omega t}\, d\omega$ there is an uncertainty in the definition of $A(\omega)$. If $A(\omega)$ is replaced by $A(\omega)\ e^{-i\gamma(\omega)}$ and $\psi_\omega(\vec{r})$ replaced by $\psi_\omega(\vec{r})\ e^{i\gamma(\omega)}$, where γ is a real function of ω, we see that $\psi_\omega(\vec{r})$ still satisfies $H\psi_\omega(r) = \hbar\omega\psi_\omega(r)$ and equation 2. We say $A(\omega)$ has $\vec{r}_0$ phasing if $\psi_\omega(\vec{r})$ is phased so that $\psi_\omega(\vec{r}_0)$ is real and positive for all ω. For any given wavefunction $\psi(r,t)$, this automatically determines the phasing of $A(\omega)$, and thus $A(\omega)$ is uniquely defined.

Energy Degeneracy

In solving the equation $H\psi_\omega(\vec{r}) = \hbar\omega\psi_\omega(\vec{r})$ we may have a number (in some cases infinitely many) linearly independent solutions. For a given wavefunction $\psi(r,t)$ only one solution of this equation contributes to the superposition over ω_s in $\psi(\vec{r},t)$. A solution ψ'_ω of $H\psi'_\omega = \hbar\omega\psi'_\omega$ which is orthogonal to ψ_ω, the contributing solution, is also orthogonal to $\psi(\vec{r},t)$.

Given a wavefunction $\psi(\vec{r},t)$ expanded in energy eigenfunctions as in equation (1), let us assume $\vec{r}_0$ phasing of these energy eigenfunctions. Then the energy distribution amplitude $A(\omega)$ is uniquely determined. Extend the definition of $A(\omega)$ for $-\infty < \omega < 0$ so that $A(\omega) = 0$ for $\omega < 0$. $A(\omega)$ is called the energy amplitude function for $\vec{r}_0$ phasing of the particle with position wavefunction $\psi(r,t)$. We define $T(t)$ as the time amplitude function of the particle by the Fourier transform relation

$$T(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(\omega)\, e^{-i\omega t}\, d\omega \ .$$

We thus have the following equivalences of operators

(a) Position and momentum wavefunctions (one dimension)

$$x \sim i\,\frac{\partial}{\partial k} \quad , \quad \psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k,t)\, e^{ikx}\, dk \ ,$$

$$k \sim -i\,\frac{\partial}{\partial x} \quad , \quad \phi(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x,t)\, e^{-ikx}\, dx \ .$$

For three dimensions we have:

$$\vec{r} \sim i\Delta_{\vec{k}} \quad ,$$

$$\vec{k} \sim -i\Delta_{\vec{r}} \quad , \quad \psi(r,t) = \frac{1}{(2\pi)^{3/2}} \int_{\text{space}} \phi(\vec{k},t)\, e^{i\vec{k}\cdot\vec{r}}\, d^3\vec{k} \quad .$$

(b) Energy and time amplitude functions.

$$\omega \sim i\frac{\partial}{\partial t} \quad , \quad A(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} T(t)\, e^{i\omega t}\, dt \quad ,$$

$$t \sim -i\frac{\partial}{\partial \omega} \quad , \quad T(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(\omega)\, e^{-i\omega t}\, d\omega \quad .$$

Observe that the position or momentum wavefunction completely determines all knowledge of the particle, but this is by no means true for the energy (or time) amplitude functions. Specifying the position wavefunction determines the energy amplitude function but not conversely. Also, observe that the energy amplitude function may depend on $\vec{r}_0$.

Using the energy and time wavefunctions, we can establish the time-energy uncertainty relation as a direct consequence of the general theorem on conjugate Hermitian operators. Observe that $[\omega,t] = i$ and so

$$\Delta\omega\Delta t \geq \frac{1}{2} \quad \text{where} \quad (\Delta\omega)^2 = \langle(\omega-\langle\omega\rangle)^2\rangle = \langle\omega^2\rangle - \langle\omega\rangle^2$$

and

$$(\Delta t)^2 = \langle(t-\langle t\rangle)^2\rangle = \langle t^2\rangle - \langle t\rangle^2 \quad .$$

Interpretation of the Time Amplitude Function

A particle may be detected by placing a screen in a specified position. Consider, as an example, a free particle in one dimension with a localized positive momentum distribution (i.e. $\phi(k,t) = 0$ for $k < 0$).

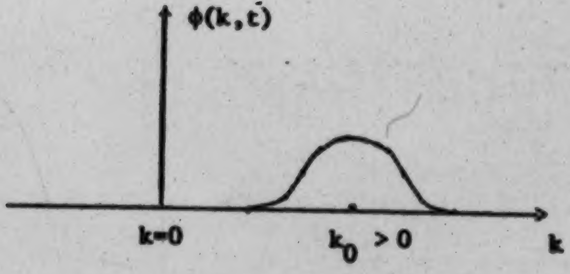

Figure 10

Positive Momentum Disbtribution

This particle is moving in the positive x direction. Suppose we place a screen at $x = x_0$, and we ask at what time does the particle hit the screen. We may make a series of measurements and find a distribution of different times. The probability that the particle hits the screen at a time between t and $t+dt$ is $|T(t)|^2\,dt$ where $T(t)$ is the time amplitude function derived from x_0 phasing.

Example - Free Particle with Positive Momentum

Let us explicitly obtain $T(t)$ for the free particle in one dimension with positive momentum. The wavefunction is

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k,0)\, e^{ikx}\, e^{\frac{-i\hbar k^2 t}{2m}}\, dk$$

where $\phi(k,0) = 0$ for $k < 0$. Consequently the above integral need only run from 0 to ∞.

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{0}^{\infty} \phi(k,0)\, e^{ikx}\, e^{\frac{-i\hbar k^2 t}{2m}}\, dk \quad .$$

The Hamiltonian H is $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$. Let us first obtain $\psi_\omega(x)$. We note that $H\psi_\omega(x) = \hbar\omega\psi_\omega(x)$ so that

$$\psi_\omega(x) = \alpha(\omega)\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,x} + \beta(\omega)\, e^{-i\sqrt{\frac{2m\omega}{\hbar}}\,x} \quad .$$

We can see that $\beta(\omega) = 0$ since the superposition for $\psi(x,t)$ involves only positive momenta $\hbar k$. In the integral

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{0}^{\infty} \phi(k,0)\, e^{ikx}\, e^{\frac{-i\hbar k^2 t}{2m}}\, dk$$

make the substitution $\omega = \frac{\hbar k^2}{2m}$ and change the variable of integration to get

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{0}^{\infty} \phi\left(\sqrt{\frac{2m\omega}{\hbar}}, 0\right) e^{i\sqrt{\frac{2m\omega}{\hbar}}\,x}\, e^{-i\omega t} \sqrt{\frac{m}{2\omega\hbar}}\, d\omega \quad . \qquad (5)$$

Now let us determine $\alpha(\omega)$ in the equation $\psi_\omega(x) = \alpha(\omega)\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,x}$. First of all, is the normalization condition $\int_{-\infty}^{\infty} \psi^*_{\omega_1}(x)\, \psi_{\omega_2}(x)\, dx = \delta(\omega_1 - \omega_2)$.

This implies that $|\alpha(\omega)|^2 = \frac{1}{2\pi}\sqrt{\frac{m}{2\omega\hbar}}$. For x_0 phasing we set $\alpha(\omega) = \sqrt[4]{\frac{m}{8\pi^2\omega\hbar}}\, e^{-i\sqrt{\frac{2m\omega}{\hbar}}\,x_0}$. This means that

$$\psi_\omega(x) = \sqrt[4]{\frac{m}{8\pi^2\omega\hbar}}\; e^{i\sqrt{\frac{2m\omega}{\hbar}}\,(x-x_0)} \quad . \tag{6}$$

If we compare (5) and (6) with (1) we can extract $A(\omega)$ as

$$A(\omega) = \sqrt[4]{\frac{m}{2\omega\hbar}}\;\phi\left(\sqrt{\frac{2m\omega}{\hbar}},\, 0\right)\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,x_0} \quad . \tag{7}$$

Equation (7) defines the energy amplitude function $A\,(\omega)$ for $\omega > 0$. We define $A(\omega) = 0$ for $\omega \leq 0$.

The time amplitude function is determined from (7) by the Fourier transform

$$T(t) = \frac{1}{\sqrt{2\pi}}\int_0^\infty \sqrt[4]{\frac{m}{2\omega\hbar}}\;\phi\left(\sqrt{\frac{2m\omega}{\hbar}}\,,\, 0\right)\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,x_0}\; e^{-i\omega t}\; d\omega \quad .$$

Now let us change the variable of integration back to $k = \sqrt{\frac{2m\omega}{\hbar}}$. Then

$$T(t) = \frac{1}{\sqrt{2\pi}}\int_0^\infty \sqrt{\frac{m}{\hbar k}}\;\phi(k,0)\; e^{ikx_0}\; e^{\frac{-i\hbar k^2 t}{2m}}\;\frac{\hbar k\,dk}{m} \quad ,$$

or

$$T(t) = \frac{1}{\sqrt{2\pi}}\int_0^\infty \sqrt{\frac{\hbar k}{m}}\;\phi(k,0)\; e^{ikx_0}\; e^{\frac{-i\hbar k^2 t}{2m}}\; dk \quad . \tag{8}$$

Let us write $T(t,x_0)$ for $T(t)$ with x_0 phasing. We see that $i\hbar \frac{\partial}{\partial t} T(t,x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} T(t,x)$, i.e. $T(t,x)$ satisfies the Schrödinger equation for a free particle. Also, observe that $\int_{-\infty}^{\infty} |T(t,x)|^2 dt = 1$ for all x . Since $T(t,x)$ satisfies the Schrödinger equation, we have its time dependence as

$$T(t,x) = \frac{(1-i)}{2}\sqrt{\frac{m}{\pi\hbar(t-t_0)}}\int_{-\infty}^{\infty} T(t_0,\bar{x}) \exp\left(\frac{im(x-\bar{x})^2}{2\hbar(t-t_0)}\right) d\bar{x} .$$

In terms of the momentum wavefunction, $T(t,x)$ is

$$T(t,x) = \frac{1}{\sqrt{2\pi}}\int_0^{\infty}\sqrt{\frac{\hbar k}{m}}\, \phi(k,t)\, e^{ikx}\, dk \quad .$$

Alternatively

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_0^{\infty} \phi(k,t)\, e^{ikx}\, dk \quad .$$

Apply fractional differentiation with respect to x to degree $\frac{1}{2}$. $D_x^{1/2}\, \psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_0^{\infty} \phi(k,t)\, (ik)^{1/2}\, e^{ikx}\, dx$. Comparison gives us the important connection between the position and time wavefunctions,

$$T(t,x) = (1-i)\sqrt{\frac{\hbar}{2m}}\; D_x^{1/2}\, \psi(x,t) \quad . \qquad (9)$$

This provides the required connection between the time and position wavefunctions, and provides the obvious method for calculating the time wavefunction.

With respect to the class of functions considered, we have the operator equivalence $i\hbar D_t' = -\frac{\hbar^2}{2m} D_x^2$. This means that $D_t^{\alpha} = (\frac{i\hbar}{2m})^{\alpha} D_x^{2\alpha}$ and $D_x^{\beta} = (\frac{2m}{i\hbar})^{\beta/2} D_t^{\beta/2}$. Thus the operator $D_x^{1/2}$ in (9) may be transformed into $D_t^{1/4}$. Also, $\psi(x,t)$ can be determined from $T(t,x)$ by means of the operator $D_x^{-1/2}$. Thus if $T(t,x)$ is known for all t and all x , all knowledge of the particle is determined.

Let us use (9) to express $T(t,x)$ in terms of $\psi(x,t)$ using $D_t^{1/4}$. We get

$$T(t,x) = \sqrt{\frac{\hbar}{im}}\, D_x^{1/2}\, \psi(x,t)$$

$$= \sqrt{\frac{\hbar}{im}}\, (\frac{2m}{i\hbar})^{1/4}\, D_t^{1/4}\, \psi(x,t) .$$

Thus

$$T(t,x) = (\frac{2i\hbar}{m})^{1/4}\, D_t^{1/4}\, \psi(x,t)$$

$$= (\frac{2}{m})^{1/4} [i\hbar D_t]^{1/4}\, \psi(x,t) = (\frac{2}{m})^{1/4}\, H^{1/4}\, \psi(x,t) .$$

$$T(t,x) = (\frac{2}{m})^{1/4}\, H^{1/4}\, \psi(x,t) \quad . \tag{10}$$

In (10) H is the Hamiltonian operator.

For fractional powers of a Hermitian operator, we assume all the eigenvalues are nonnegative. $H^{1/4}$ has the same eigenfunctions as H and the eigenvalues are the positive real fourth roots of the eigenvalues of H . Equation (10) gives the free particle time wavefunction, where H is the free particle Hamiltonian.

Normalization of the Free Particle Time Wavefunction in Time

The time wavefunction $T(t,x)$ satisfies $i\hbar \frac{\partial}{\partial t} T(t,x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} T(t,x)$ and consequently has the time dependent form

$$T(t,x) = \frac{(1-i)}{2}\sqrt{\frac{m}{\pi\hbar(t-t_0)}}\int_{-\infty}^{\infty} T(t_0,\bar{x})\, \exp\left(\frac{im(x-\bar{x})^2}{2\hbar(t-t_0)}\right) d\bar{x} \quad .$$

First of all, let us examine the consequences of time normalization, namely $\int_{-\infty}^{\infty} |T(t,x)|^2\, dt = 1$. Recall that $D_x^{\alpha}\,\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} (ik)^{\alpha} e^{ikx}\, dk$ and $D_x^{-1}\,\delta(x) = \frac{1}{2}\,\mathrm{sgn}\, x$, $D_x^{-2}\,\delta(x) = \frac{1}{2}\,|x|$ (even and odd function symmetry).

Thus

$$1 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} + \frac{1}{2}\,\frac{m}{\pi\hbar(t-t_0)}\, T^*(t_0,\bar{x})T(t_0,\bar{\bar{x}})\exp\left(\frac{-im(x-\bar{x})^2}{2h(t-t_0)}\right)\exp\left(\frac{im(x-\bar{\bar{x}})^2}{2h(t-t_0)}\right) dt\,d\bar{x}\,d\bar{\bar{x}} \;,$$

and

$$1 = +\frac{m}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} T^*(t_0,\bar{x})T(t_0,\bar{\bar{x}})\left[\int_{-\infty}^{\infty} \exp\left(\frac{im[(x-\bar{\bar{x}})^2-(x-\bar{x})^2]}{2h(t-t_0)}\right)\frac{dt}{t-t_0}\right] d\bar{x}\, d\bar{\bar{x}} \quad .$$

Consider the t integral separately. We have

$$\int_{-\infty}^{\infty} \exp\left(\frac{im(\bar{\bar{x}}-\bar{x})(\bar{\bar{x}}+\bar{x}-2x)}{2\hbar t}\right)\frac{dt}{t} = \left[\int_{-\infty}^{0^-}+\int_{0^+}^{\infty}\right] \exp\left(\frac{im[(x-\bar{\bar{x}})^2-(x-\bar{x})^2]}{2\hbar t}\right)\frac{dt}{t}$$

$$= \left[\int_{0^-}^{-\infty}+\int_{+\infty}^{0^+}\right] \exp\left(\frac{im}{2h}\,[(x-\bar{\bar{x}})^2-(x-\bar{x})^2]u\right)\left(-\frac{du}{u}\right)$$

$$= \int_{-\infty}^{\infty} \exp\left(\frac{im}{2\hbar}\left[(x-\bar{\bar{x}})^2-(x-\bar{x})^2\right]u\right) \frac{du}{u}$$

$$= \int_{-\infty}^{\infty} e^{iku} \frac{du}{u}$$

where $k = \frac{m}{2\hbar}\left[(x-\bar{\bar{x}})^2-(x-\bar{x})^2\right]$. Observe that $\int_{-\infty}^{\infty} e^{iku} \frac{du}{u} = i\,\pi \operatorname{sgn} k$.

Thus the t integral equals $i\pi \operatorname{sgn}\left[(x-\bar{\bar{x}})^2-(x-\bar{x})^2\right]$ since $\frac{m}{2\hbar}$ is positive. Thus we have

$$1 = \frac{im}{2\hbar} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} T^*(t_0,\bar{x})T(t_0,\bar{\bar{x}}) \operatorname{sgn}\left[(x-\bar{\bar{x}})^2-(x-\bar{x})^2\right] d\bar{x}\, d\bar{\bar{x}} \quad . \tag{11}$$

(11) holds for all t_0 and all x and is a method of reformulating the normalization condition on $T(t,x)$.

If we evaluate $\langle t\rangle = \int_{-\infty}^{\infty} T^*(t,x)t\, T(t,x)\, dt$ this way we get $\langle t\rangle_x = t_0 - \frac{m^2}{4\hbar^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} T^*(t_0,\bar{x})T(t_0,\bar{\bar{x}})\left|(x-\bar{\bar{x}})^2-(x-\bar{x})^2\right| d\bar{x}\, d\bar{\bar{x}}$. Let us use the expression $T(t,x) = \frac{1}{\sqrt{2\pi}}\int_0^{\infty}\sqrt{\frac{\hbar k}{m}}\,\phi(k,0)\, e^{ikx}\, e^{\frac{-i\hbar k^2 t}{2m}}\, dk$, to calculate $\langle t\rangle$. As an integral over ω , $T(t,x)$ reads as

$$T(t,x) = \frac{1}{\sqrt{2\pi}}\int_0^{\infty}\left(\frac{m}{2\omega\hbar}\right)^{1/4}\phi\left(\sqrt{\frac{2m\omega}{\hbar}},0\right) e^{i\sqrt{\frac{2m\omega}{\hbar}}\,x}\, e^{-i\omega t}\, d\omega \quad ,$$

so

$$\langle t\rangle = \int_{-\infty}^{\infty} T^*(t,x)t\, T(t,x)dt = \int_0^{\infty} A^*(\omega,x)\left[-i\frac{\partial}{\partial\omega}\right] A(\omega,x)\, d\omega \quad .$$

We note that $A(\omega,x) = (\frac{m}{2\omega\hbar})^{1/4}\ \phi(\sqrt{\frac{2m\omega}{\hbar}}, 0)\ e^{i\sqrt{\frac{2m\omega}{\hbar}}x}$. We can transform the variable of integration from ω to $k = \sqrt{\frac{2m\omega}{\hbar}}$.

$$\langle t\rangle = \int_0^\infty A^*(\frac{\hbar k^2}{2m}, x)[-i\frac{\partial}{\partial k}]\ A(\frac{\hbar k^2}{2m}, x)\ \frac{dk}{d\omega}\,d\omega \quad .$$

We note that $A(\frac{\hbar k^2}{2m}, x) = (\frac{m}{\hbar k})^{1/2}\ \phi(k,0)\ e^{ikx}$. Thus

$$\langle t\rangle_x = \int_0^\infty (\frac{m}{\hbar k})^{1/2}\ \phi^*(k,0)e^{-ikx}\ [-i\frac{\partial}{\partial k}]\{(\frac{m}{\hbar k})^{1/2}\ \phi(k,0)e^{ikx}\}\ dk$$

$$= \int_0^\infty \{\frac{i}{2}\frac{m}{\hbar k^2}\ |\phi(k,0)|^2 - i(\frac{m}{\hbar k})\phi^*(k,0)\phi'(k,0) + x(\frac{m}{\hbar k})|\phi(k,0)|^2\}\ dk$$

$$= \langle\frac{i}{2}\frac{m}{\hbar k^2} - \frac{im}{\hbar k}\frac{\partial}{\partial k} + \frac{xm}{\hbar k}\rangle_{t=0}$$

on the momentum function. Observe that $\frac{d}{dx}(\langle t\rangle_x) = \frac{m}{\hbar}\langle\frac{1}{k}\rangle_{t=0}$ a constant independent of x . For very narrow k distributions about k_0 we estimate $\langle\frac{1}{k}\rangle_{t=0} = \frac{1}{k_0}$ where the narrow momentum distribution is centred at k_0 . Then $\frac{d}{dx}(\langle t\rangle_x) = \frac{m}{\hbar k_0} = \frac{1}{v}$ where v is the propogation velocity of the particle, $v = \frac{\hbar\langle k\rangle}{m}$. This is consistent with the notion that if a particle is stopped at a position x_0 , $|T(t,x_0)|^2dt$ is the probability of measuring the time of impact between t and $t+dt$. Observe that $\langle t\rangle_{x=0} = \langle\frac{i}{2}\frac{m}{\hbar k^2} - \frac{im}{\hbar k}\frac{\partial}{\partial k}\rangle_{t=0}$. This gives the absolute position for setting of the clock. The Hermitian operator $\frac{i}{2}\frac{m}{\hbar k^2} - \frac{im}{\hbar k}\frac{\partial}{\partial k}$ is the time setting operator for the free particle. We can give an intuitive argument to illustrate why the time setting corresponds with expectations for a narrow momentum distribution. We note that $\langle x\rangle_t = \langle x\rangle_{t=0} + vt$ where $v = \frac{\hbar k_0}{m}$. Thus we expect $\langle t\rangle_{x=0} = -\frac{\langle x\rangle_{t=0}}{v} = -\frac{m\langle x\rangle_{t=0}}{\hbar k_0}$. Now let us look at $\langle \frac{i}{2}\frac{m}{\hbar k^2} - \frac{im}{\hbar k}\frac{\partial}{\partial k}\rangle_{t=0}$ and ignore the term $\frac{i}{2}\frac{m}{\hbar k^2}$ which appears simply to make the operator Hermitian, and has imaginary expectation values. We estimate (for narrow k distribution about k_0), using the operator equivalence $x \sim i\frac{\partial}{\partial k}$ that $\langle -\frac{im}{\hbar k}\frac{\partial}{\partial k}\rangle_{t=0} \approx -\frac{m}{\hbar k_0}\langle x\rangle_{t=0} = \langle t\rangle_{x=0}$. This hopefully, makes plausible the time setting equation $\langle t\rangle_{x=0} = \langle \frac{i}{2}\frac{m}{\hbar k^2} - \frac{im}{\hbar k}\frac{\partial}{\partial k}\rangle_{t=0}$ and provides a connection between the physical interpretation of $|T(t,x)|^2$ and its mathematical construction.

In general, for an arbitrary Hamiltonian (not a free particle) $T(t,\vec{r})$ does not satisfy the Schrödinger equation that $\psi(\vec{r},t)$ does, namely $i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = H\,\psi(\vec{r},t)$. One can however obtain $T(t,\vec{r})$ from $\psi(\vec{r},t)$ by an appropriate transformation.

Since $\psi(\vec{r},t)$ is completely determined from $\psi(\vec{r},0)$ let us start with $\psi(\vec{r},0)$. We have

$$\psi(\vec{r},t) = \int_0^\infty A(\omega,\vec{r}_0)\,\psi_{\omega,\vec{r}_0}(\vec{r})\,e^{-i\omega t}\,d\omega \quad \text{for all } \vec{r}_0$$

$$T(t,\vec{r}_0) = \frac{1}{\sqrt{2\pi}}\int_0^\infty A(\omega,\vec{r}_0)\,e^{-i\omega t}\,d\omega$$

$$A(\omega,\vec{r}_0) = \int_{\text{space}} \psi^*_{\omega,\vec{r}_0}(\vec{r})\,\psi(\vec{r},0)\,d\vec{r}\ .$$

Note that $H\,\psi_{\omega,\vec{r}_0}(\vec{r}) = \hbar\omega\psi_{\omega,\vec{r}_0}(\vec{r})$ and $\psi_{\omega,\vec{r}_0}(\vec{r}_0) \geq 0$. $|A(\omega,\vec{r}_0)|^2$

depends only on ω and not on $\vec{r}_0$. Also $\int_{\substack{\text{all}\\ \text{space}}} \psi^*_{\omega_1,\vec{r}_0}(\vec{r})\psi_{\omega_2,\vec{r}_0}(\vec{r})d\vec{r} = \delta(\omega_1-\omega_2)$. We have

$$T(t,\vec{r}_0) = \frac{1}{\sqrt{2\pi}}\int_0^\infty \int_{\text{space}} \psi^*_{\omega,\vec{r}_0}(\vec{r})\, e^{-i\omega t}\psi(\vec{r},0)\, d\vec{r}\, d\omega \quad .$$

Alternatively, using

$$A(\omega,\vec{r}_0) = e^{i\omega t_0}\int_{\text{space}} \psi^*_{\omega,\vec{r}_0}(\vec{r})\psi(\vec{r},t_0)\, d\vec{r}$$

we get

$$T(t,\vec{r}_0) = \frac{1}{\sqrt{2\pi}}\int_0^\infty \int_{\text{space}} \psi^*_{\omega,\vec{r}_0}(\vec{r})\, e^{-i\omega(t-t_0)}\psi(\vec{r},t_0) d\vec{r}\, d\omega \quad .$$

Note that $|\psi_{\omega,\vec{r}_0}(\vec{r})|$ is indpendent of $\vec{r}_0$. Also, knowledge of $T(t,\vec{r}_0)$ may not be sufficient to determine $\psi(\vec{r},t_0)$.

Eigenfunctions and Eigenvalues for the Free Particle Time Setting Operator

We saw that for a free particle,

$$\langle t\rangle_{x_0} = t_0 + \left\langle \frac{i}{2}\frac{m}{\hbar k^2} - \frac{im}{\hbar k}\frac{\partial}{\partial k} + \frac{x_0 m}{\hbar k}\right\rangle_{t=t_0}$$

on the momentum wavefunction $\phi(k,t_0)$. Alternatively, we can move the constant inside the expectation and obtain

$$\langle t\rangle_{x_0} = \langle t_0 + \frac{1}{2}\frac{m}{\hbar k^2} - \frac{im}{\hbar k}\frac{\partial}{\partial k} + \frac{x_0 m}{\hbar k}\rangle_{t=t_0} .$$

The operator $t_0 + \frac{1}{2}\frac{m}{\hbar k^2} - \frac{im}{\hbar k}\frac{\partial}{\partial k} + \frac{x_0 m}{\hbar k}$ is called the time operator for the free particle in one dimension, and it operates on a restricted subclass of the possible states of a system. In this case we assume the momentum distribution is positive and bounded away from $k = 0$, i.e. $\phi(k,t) = 0$ for $k < k_1$ where $k_1 > 0$.

One interesting question is to ask what are the eigenvalues and eigenfunctions for this free particle time operator. The differential equation to solve is

$$(t_0 + \frac{1}{2}\frac{m}{\hbar k^2} - \frac{im}{\hbar k}\frac{\partial}{\partial k} + \frac{x_0 m}{\hbar k}) f(k) = \lambda f(k) ,$$

or

$$t_0 f + \frac{1}{2}\frac{m}{\hbar k^2} f - \frac{im}{\hbar k}\frac{df}{dk} + \frac{x_0 m}{\hbar k} f = \lambda f .$$

Multiply through by $\frac{kdk}{f}$ and integrate to get

$$t_0 \frac{k^2}{2} + \frac{1}{2}\frac{m}{\hbar}\log k - \frac{im}{\hbar}\log f + \frac{x_0 m}{\hbar} k = \lambda \frac{k^2}{2} + \text{constant.}$$

Solving for f gives

$$f = A\, k^{1/2} \exp(\frac{i\hbar k^2}{2m}(\lambda - t_0) - i x_0 k) .$$

A is a function of λ , t_0 and x_0 . Thus

$$f_\lambda(k) = Ak^{1/2} \exp(\frac{i\hbar k^2}{2m}(\lambda - t_0) - ix_0k) \ .$$

It remains to determine the normalization conditions in order to obtain the coefficient A . Let us return to a consideration of the equation.

$$T(\lambda, x_0) = \int_0^\infty \phi(k, t_0) \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\hbar k}{m}} \exp\{ikx_0 - \frac{i\hbar k^2}{2m}(\lambda - t_0)\} \ dk$$

$$= \int_0^\infty \phi(k, t_0) f_\lambda^*(k) \ dk \ .$$

This holds if we take

$$f_\lambda(k) = \sqrt{\frac{\hbar}{2\pi m}} \ k^{1/2} \exp\{-ikx_0 + \frac{i\hbar k^2}{2m}(\lambda - t_0)\} \ ,$$

so that $A = \sqrt{\frac{\hbar}{2\pi m}}$. We write $f_\lambda(k)$ as $f_{\lambda(x_0, t_0)}(k)$ to indicate the dependence on t_0 and x_0 . Thus

$$f_{\lambda(x_0, t_0)}(k) = \sqrt{\frac{\hbar}{2\pi m}} \ k^{1/2} \exp\{-ikx_0 + \frac{i\hbar k^2}{2m}(\lambda - t_0)\} \tag{12}$$

is an eigenfunction of the time operator $t_0 + \frac{1}{2}\frac{m}{\hbar k^2} - \frac{im}{\hbar k}\frac{\partial}{\partial k} + \frac{x_0 m}{\hbar k}$, with eigenvalue λ . Also we have

$$T(\lambda, x_0) = \int_0^\infty \phi(k, t_0) f^*_{\lambda(x_0, t_0)}(k) \ dk \ . \tag{13}$$

Now let us take (13) and multiply by $f_{\lambda(x_0, t_0)}(k')$ and integrate over λ .

$$\int_{-\infty}^{\infty} T(\lambda,x_0) f_{\lambda(x_0,t_0)}(k')d\lambda = \int_0^{\infty} \phi(k,t_0)[\int_{-\infty}^{\infty} f^*_{\lambda(x_0,t_0)}(k) f_{\lambda(x_0,t_0)}(k')d\lambda]\, dk ,$$

$$= \phi(k',t_0) .$$

We can show $\delta(k'-k) = \int_{-\infty}^{\infty} f^*_{\lambda(x_0,t_0)}(k) f_{\lambda(x_0,t_0)}(k')d\lambda$ for $k, k' > 0$ and so

$$\phi(k,t_0) = \int_{-\infty}^{\infty} T(\lambda,x_0) f_{\lambda(x_0,t_0)}(k)\, d\lambda . \tag{14}$$

We must always be careful to note that only positive momenta k are allowed in the transformation between momentum wave function and time amplitude function.

General Results - Time Operator and Eigenfunctions

The domain of a time operator. For a given Hamiltonian H the time operator which is conjugate to H will not in general be unique, nor will its domain cover the entire Hilbert space in consideration. By examining the general theory, we can see to what extent this is true.

For the given Hamiltonian H, let us look at all energy eigenfunctions ψ_ω such that $H\psi_\omega = \hbar\omega\psi_\omega$ over all possible ω. The sp ectrum S of H is the range of all possible ω for which this equation has a nontrivial solution ψ_ω. For any given ω there may be more than one linearly independent energy eigenfunction.

Definition: A Time Domain D is a subspace of the Hilbert space spanned by a collection of ψ_ω such that for each $\omega \in S$ exactly one function ψ_ω satisfying $H\psi_\omega = \hbar\omega\psi_\omega$ is in D .

Consequently every energy level has a representative in D as a subspace of D of dimension 1. There are no energy degeneracies in D .

Example: An example of a time domain consider the free particle with positive momentum distribution in one dimension.

For a given Hamiltonian H it is often possible to construct many time domains. To each time domain D there corresponds a time operator conjugate to H with domain D . In general we assume H is the Hamiltonian for a particle moving through a local potential. Consequently S is the spectrum of positive ω . For $\psi_\omega \in D$ we generally require that ψ_ω depends continuously on ω .

A position wavefunction $\psi(\vec{r},t)$ can be expanded in energy eigenfunctions as $\psi(\vec{r},t) = \int_0^\infty A(\omega)\psi_\omega(\vec{r})\, e^{-i\omega t}\, d\omega$ (equation (1)). The normalized functions $\psi_\omega(\vec{r})$ satisfying (2) form a basis for a time domain D . $\psi(\vec{r},t)$ is an element of D for all time t .

Let us assume we are working in a fixed time domain D spanned by the functions $\psi_\omega(\vec{r})$. Let

$$\psi_{\omega,\vec{r}_0}(\vec{r}) = \frac{\psi_\omega(\vec{r})\psi^*_\omega(\vec{r}_0)}{|\psi_\omega(\vec{r}_0)|} = \frac{\psi_\omega(\vec{r})}{\psi_\omega(\vec{r}_0)}\,|\psi_\omega(\vec{r}_0)| \quad .$$

Then we have

$$T(t,\vec{r}_0) = \int_{\text{space}} \left[\frac{1}{\sqrt{2\pi}} \int_0^\infty \psi^*_{\omega,\vec{r}_0}(\vec{r}) e^{-i\omega(t-t_0)} d\omega\right] \psi(\vec{r},t_0)\, d\vec{r}$$

$$= \int_{\text{space}} f^*_{\vec{r}_0,(t-t_0)}(\vec{r})\psi(\vec{r},t_0)\, d\vec{r} \quad ,$$

where $f_{\vec{r}_0,(t-t_0)}(\vec{r}) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \psi_{\omega,\vec{r}_0}(\vec{r})\, e^{i\omega(t-t_0)} d\omega$. This expansion can be inverted as $\psi(\vec{r},t_0) = \int_{-\infty}^\infty f_{\vec{r}_0(t'-t_0)}(\vec{r})\; T(t',\vec{r}_0)\, dt'$. There is a unique one to one relation between ψ and T as long as ψ remains in the time domain D . Observe that

$$T(t,\vec{r}_0) = \int_{\text{space}} f^*_{\vec{r}_0(t-t_0)}(\vec{r})\, d\vec{r} \int_{-\infty}^\infty f_{\vec{r}_0(t'-t_0)}(\vec{r}) T(t',\vec{r}_0)\, dt'$$

$$= \int_{-\infty}^\infty dt'\; T(t',\vec{r}_0) \int_{\text{space}} f^*_{\vec{r}_0(t-t_0)}(\vec{r})\; f_{\vec{r}_0(t'-t_0)}(\vec{r})\, d\vec{r}$$

$$= \int_{-\infty}^\infty dt'\; T(t',\vec{r}_0)\delta(t'-t) \quad .$$

This means $\delta(t'-t) = \int_{\text{space}} f^*_{\vec{r}_0(t-t_0)}(\vec{r})\; f_{\vec{r}_0(t'-t_0)}(\vec{r})\, d\vec{r}$. This can be verified by substitution if one remembers that only $\omega > 0$ is allowed in the distribution of energies. This in turn restricts the admissible functions $T(t,\vec{r}_0)$ as functions of t , so the transformation above has the same properties as $\delta(t'-t)$ on the admissible time amplitude functions.

Let us examine this transformation which we called "$\delta(t'-t)$" in some more detail to see exactly how it acts on time amplitude functions.

Observe that

$$\int_{\text{space}} f^{*}_{\vec{r}_0(t-t_0)}(\vec{r})\ f_{\vec{r}_0(t'-t_0)}(\vec{r})\ d\vec{r} =$$

$$= \int_{\text{space}} \left(\frac{1}{\sqrt{2\pi}} \int_0^\infty \psi^{*}_{\omega,\vec{r}_0}(\vec{r})\ e^{-i\omega(t-t_0)} d\omega\right)\left(\frac{1}{\sqrt{2\pi}} \int_0^\infty \psi_{\bar{\omega},\vec{r}_0}(\vec{r}) e^{i\bar{\omega}(t'-t_0)} d\bar{\omega}\right) d\vec{r} \ .$$

$$= \frac{1}{2\pi} \int_0^\infty \int_0^\infty \delta(\omega-\bar{\omega}) e^{i\bar{\omega}(t'-t_0)-i\omega(t-t_0)} d\omega d\bar{\omega} = \frac{1}{2\pi} \int_0^\infty e^{i\omega(t'-t)}\ d\omega \ .$$

The last term would be recognized as $\delta(t-t')$ had the integral extended over $-\infty$ to ∞ in ω. In fact it behaves like a δ transformation (identity) over a restricted subdomain which precisely includes the time amplitude functions.

Let us evaluate $\int_{-\infty}^{\infty} dt'\ T(t',\vec{r}_0)\left(\frac{1}{2\pi} \int_0^\infty e^{i\omega(t'-t)} d\omega\right)$. Performing the integration over t' and using the Fourier transform relation $A(\omega,\vec{r}_0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} T(t',\vec{r}_0) e^{i\omega t'}\ dt'$ we get the above integral equals $\frac{1}{\sqrt{2\pi}} \int_0^\infty A(\omega,\vec{r}_0)\ e^{-i\omega t}\ d\omega$. But we know $A(\omega,\vec{r}_0) = 0$ for $\omega < 0$ and this equals $\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(\omega,\vec{r}_0) e^{-i\omega t}\ d\omega$ which is simply $T(t,\vec{r}_0)$. This proves the required inversion relation.

The Time Operator

We wish to have $f_{\vec{r}_0(t-t_0)}(\vec{r})$ as eigenfunctions of the time operator $\tau_{\vec{r}_0,t_0}$ with eigenvalue t. $\tau_{\vec{r}_0,t_0}$ operates on position wavefunctions in the time domain D. The wavefunction it operates on is $\psi(\vec{r},t_0)$ the position wavefunction at time t_0. It is used to measure time of arrival at $\vec{r}_0$. In this way we could generalize the results already considered for a free particle in one dimension with a positive energy and momentum distribution. Let us examine the expected value of time of arrival at $\vec{r}_0$.

$$\langle t\rangle_{\vec{r}_0} = \int_{-\infty}^{\infty} t\,|T(t,\vec{r}_0)|^2\,dt = \int_{-\infty}^{\infty} T^*(t,\vec{r}_0)\,t\,T(t,\vec{r}_0)\,dt$$

$$= \int_{-\infty}^{\infty}\left[\int_{\text{space}} f_{\vec{r}_0(t-t_0)}(\vec{r}\,')\,\psi^*(\vec{r}\,',t_0)\,d\vec{r}\,'\right] t \left[\int_{\text{space}} f^*_{\vec{r}_0(t-t_0)}(\vec{r})\,\psi(\vec{r},t_0)\,d\vec{r}\right] dt$$

$$= \int_{\text{space}} \psi^*(\vec{r},t_0)\,\underset{\substack{\uparrow\\ \text{operator}}}{\tau_{\vec{r}_0,t_0}}\,\psi(\vec{r},t_0)\,d\vec{r}$$

$$= \int_{\text{space}}\int_{\text{space}} \psi^*(\vec{r}\,',t_0)\,\underbrace{\tau_{\vec{r}_0,t_0}(\vec{r}\,',\vec{r})}_{\substack{\uparrow\\ \text{kernel.}}}\,\psi(\vec{r},t_0)\,d\vec{r}\,d\vec{r}\,' \quad .$$

By comparison we obtain the kernel as

$$T_{\vec{r}_0,t_0}(\vec{r}',\vec{r}) = \int_{-\infty}^{\infty} t\, f_{\vec{r}_0(t-t_0)}(\vec{r}')\, f^*_{\vec{r}_0(t-t_0)}(\vec{r})\, dt$$

$$= \int_{-\infty}^{\infty} t\,dt\Big(\frac{1}{\sqrt{2\pi}}\int_0^{\infty} \psi_{\omega,\vec{r}_0}(\vec{r}')e^{i\omega(t-t_0)}\,d\omega\Big)\Big(\frac{1}{\sqrt{2\pi}}\int_0^{\infty} \psi^*_{\bar{\omega},\vec{r}_0}(\vec{r})e^{-i\bar{\omega}(t-t_0)}\,d\bar{\omega}\Big)$$

$$= \int_0^{\infty}\int_0^{\infty} \psi_{\omega,\vec{r}_0}(\vec{r}')\psi^*_{\bar{\omega},\vec{r}_0}(\vec{r})\,d\omega\, d\bar{\omega}\underset{\overset{\uparrow}{-i\delta'(\omega-\bar{\omega})}}{\Big(\frac{1}{2\pi}\int_{-\infty}^{\infty} t\, e^{i(\omega-\bar{\omega})t}dt\Big)}\, e^{i(\bar{\omega}-\omega)t_0}$$

$$= \int_0^{\infty} \psi_{\omega,\vec{r}_0}(\vec{r}')e^{-i\omega t_0}\Big(-i\,\frac{\partial}{\partial\omega}\Big)\big[\psi^*_{\omega,\vec{r}_0}(\vec{r})e^{i\omega t_0}\big]\, d\omega \;.$$

Let us apply the time operator $T_{\vec{r}_0,t_0}$ to the function $f_{\vec{r}_0(t-t_0)}(\vec{r})$.

$$\int_{\text{space}} T_{\vec{r}_0,t_0}(\vec{r}',\vec{r})\, f_{\vec{r}_0(t-t_0)}(\vec{r})\, d\vec{r}$$

$$= \int_{\text{space}} f_{\vec{r}_0(t-t_0)}(\vec{r})\, d\vec{r}\int_{-\infty}^{\infty} t'\, f_{\vec{r}_0(t'-t_0)}(\vec{r}')\, f^*_{\vec{r}_0(t'-t_0)}(\vec{r})\, dt'$$

$$= \int_{-\infty}^{\infty} t'\, f_{\vec{r}_0(t'-t_0)}(\vec{r}')dt'\;\delta(t-t') = t\, f_{\vec{r}_0(t-t_0)}(\vec{r}') \;.$$

This shows that $f_{\vec{r}_0(t-t_0)}(\vec{r})$ is an eigenfunction of $T_{\vec{r}_0,t_0}$ with eigenvalue t . We can use the expression

$$f_{\vec{r}_0(t-t_0)}(\vec{r}) = \frac{1}{\sqrt{2\pi}}\int_0^{\infty} \psi_{\omega,\vec{r}_0}(\vec{r})\, e^{i\omega(t-t_0)}\, d\omega$$

to see how $T_{\vec{r}_0,t_0}$ acts on $\psi_{\omega,\vec{r}_0}(\vec{r})$. Observe that

$$\psi_{\omega,\vec{r}_0}(\vec{r}) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f_{\vec{r}_0(t-t_0)}(\vec{r})\, e^{-i\omega(t-t_0)}\,dt \quad ,$$

and so

$$T_{\vec{r}_0,t_0}(\psi_{\omega,\vec{r}_0}(\vec{r})) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} t\, f_{\vec{r}_0(t-t_0)}(\vec{r})\, e^{-i\omega(t-t_0)}\,dt \quad .$$

Now we substitute $f_{\vec{r}_0(t-t_0)}(\vec{r}) = \frac{1}{\sqrt{2\pi}}\int_0^{\infty} \psi_{\bar{\omega},\vec{r}_0}(\vec{r})\, e^{i\bar{\omega}(t-t_0)}\,d\bar{\omega}$ to get

$$T_{\vec{r}_0,t_0}(\psi_{\omega,\vec{r}_0}(\vec{r})) = \int_0^{\infty} \psi_{\bar{\omega},\vec{r}_0}(\vec{r})\,d\bar{\omega}\; \underset{\overset{\uparrow}{-i\delta'(\bar{\omega}-\omega)=i\delta'(\omega-\bar{\omega})}}{\left(\frac{1}{2\pi}\int_{-\infty}^{\infty} t e^{i(\bar{\omega}-\omega)t}dt\right)}\; e^{i(\omega-\bar{\omega})t_0} \quad .$$

Thus

$$T_{\vec{r}_0,t_0}(\psi_{\omega,\vec{r}_0}(\vec{r})) = \int_0^{\infty} i\delta(\bar{\omega}-\omega)\,d\bar{\omega}\left(\frac{\partial}{\partial\bar{\omega}}\left[\psi_{\bar{\omega},\vec{r}_0}(\vec{r})\, e^{i(\omega-\bar{\omega})t_0}\right]\right)$$

$$= \left(t_0 + i\frac{\partial}{\partial\omega}\right)\psi_{\omega,\vec{r}_0}(\vec{r}) \quad .$$

Let us calculate $[H,T_{\vec{r}_0,t_0}]\,\psi_{\omega,\vec{r}_0}(\vec{r})$. This is given by

$$[H,T_{\vec{r}_0,t_0}]\,\psi_{\omega,\vec{r}_0}(\vec{r}) = HT_{\vec{r}_0,t_0}\psi_{\omega,\vec{r}_0}(\vec{r}) - T_{\vec{r}_0,t_0}H\psi_{\omega,\vec{r}_0}(\vec{r}) \quad .$$

This evaluation requires extreme care in order to avoid errors. Remember $T_{\vec{r}_0,t_0}$ is an operator on functions of $\vec{r}$, and not functions of ω . Consequently the equation $T_{\vec{r}_0,t_0}(\psi_{\omega,\vec{r}_0}(\vec{r})) = (t_0 + i\frac{\partial}{\partial\omega})\psi_{\omega,\vec{r}_0}(\vec{r})$ is not an equivalence of operators $\tau_{\vec{r}_0,t_0}$ and $t_0 + i\frac{\partial}{\partial\omega}$. To make this point clear, if we take a linear combination of $\psi_{\omega,\vec{r}_0}(\vec{r})$ with coefficients that are functions of ω, the operator $\tau_{\vec{r}_0,t_0}$ applied to this function works as follows.

$$\tau_{\vec{r}_0,t_0}(\psi(\vec{r},t)) = \tau_{\vec{r}_0,t_0}\left(\int_0^\infty A(\omega,\vec{r}_0)\psi_{\omega,\vec{r}_0}(\vec{r})\ e^{-i\omega t}\ d\omega\right)$$

$$= \int_0^\infty A(\omega,\vec{r}_0)\ e^{-i\omega t}[\tau_{\vec{r}_0,t_0}\psi_{\omega,\vec{r}_0}(\vec{r})]\ d\omega$$

$$= \int_0^\infty A(\omega,\vec{r}_0)\ e^{-i\omega t}[(t_0 + i\frac{\partial}{\partial\omega})\psi_{\omega,\vec{r}_0}(\vec{r})]\ d\omega \quad .$$

Observe that the differentiation with respect to ω acts only on $\psi_{\omega,\vec{r}_0}(\vec{r})$ and not on $A(\omega,\vec{r}_0)$ or $e^{-i\omega t}$.

Let us look at the two terms involved in $[H,\tau_{\vec{r}_0,t_0}]\psi_{\omega,\vec{r}_0}(\vec{r})$. First observe that

$$\tau_{\vec{r}_0,t_0}H\psi_{\omega,\vec{r}_0}(\vec{r}) = \tau_{\vec{r}_0,t_0}\ \hbar\omega\psi_{\omega,\vec{r}_0}(\vec{r})$$

$$= \hbar\omega\ \tau_{\vec{r}_0,t_0}\psi_{\omega,\vec{r}_0}(\vec{r}) \ .$$

This follows since $\tau_{\vec{r}_0,t_0}$ is an operator on functions of $\vec{r}$ and $\hbar$ and ω are constants in this operation. Hence

$$\tau_{\vec{r}_0,t_0}\ H\psi_{\omega,\vec{r}_0}(\vec{r}) = \hbar\omega(t_0 + i\frac{\partial}{\partial\omega})\ \psi_{\omega,\vec{r}_0}(\vec{r}) \ .$$

Now let us look at the opposite order of operators, namely $H\tau_{\vec{r}_0,t_0}\psi_{\omega,\vec{r}_0}(\vec{r}) = H(t_0 + i\,\frac{\partial}{\partial\omega})\psi_{\omega,\vec{r}_0}(\vec{r}) = \hbar\omega t_0\psi_{\omega,\vec{r}_0}(\vec{r}) + i\,H(\frac{\partial}{\partial\omega}\,\psi_{\omega,\vec{r}_0}(\vec{r}))$. Let us consider this last term separately.

$$H(\frac{\partial}{\partial\omega}\,\psi_{\omega,\vec{r}_0}(\vec{r})) = \lim_{d\omega\to 0} H\left(\frac{\psi_{\omega+d\omega,\vec{r}_0}(\vec{r}) - \psi_{\omega,\vec{r}_0}(\vec{r})}{d\omega}\right)$$

$$= \lim_{d\omega\to 0} \frac{\hbar(\omega+d\omega)\psi_{\omega+d\omega,\vec{r}_0}(\vec{r}) - \hbar\omega\psi_{\omega,\vec{r}_0}(\vec{r})}{d\omega}$$

$$= \hbar\psi_{\omega,\vec{r}_0}(\vec{r}) + \hbar\omega\,\frac{\partial}{\partial\omega}\,\psi_{\omega,\vec{r}_0}(\vec{r}) \quad .$$

Consequently, we have

$$H\tau_{\vec{r}_0,t_0}\psi_{\omega,\vec{r}_0}(\vec{r}) = \hbar\omega t_0\psi_{\omega,\vec{r}_0}(\vec{r}) + i\hbar\psi_{\omega,\vec{r}_0}(\vec{r}) + i\hbar\omega\,\frac{\partial}{\partial\omega}\,\psi_{\omega,\vec{r}_0}(\vec{r}) \quad .$$

From these operator composition results we obtain

$$[H,\tau_{\vec{r}_0,t_0}]\psi_{\omega,\vec{r}_0}(\vec{r}) = \hbar\omega t_0\psi_{\omega,\vec{r}_0}(\vec{r}) + i\hbar\psi_{\omega,\vec{r}_0}(\vec{r}) + i\hbar\omega\,\frac{\partial}{\partial\omega}\,\psi_{\omega,\vec{r}_0}(\vec{r})$$

$$- \hbar\omega(t_0 + i\,\frac{\partial}{\partial\omega})\psi_{\omega,\vec{r}_0}(\vec{r})$$

$$= i\hbar\psi_{\omega,\vec{r}_0}(\vec{r}) \quad .$$

Thus we have $[H,\tau_{\vec{r}_0,t_0}] = i\hbar$ on the time domain D .

The Zero Rest Mass Particle in One Dimension with Positive Momentum Distribution

The Schrödinger equation corresponding to $E = cp$ is $i\hbar \frac{\partial\psi}{\partial t}(x,t) = -i\hbar c \frac{\partial\psi}{\partial x}(x,t)$ or $\frac{\partial\psi}{\partial t} = -c \frac{\partial\psi}{\partial x}$. The solution is obviously $\psi = f(x-ct)$. This can be expressed as a Fourier transform,

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_0^\infty g(k)\, e^{ik(x-ct)}\, dk = f(x-ct) \quad .$$

The momentum wavefunction is $\phi(k,t) = g(k)\, e^{-ikct}$ for $k > 0$. We have $g(k) = 0$ for $k \le 0$. ϕ satisfies $i\hbar \frac{\partial\phi}{\partial t} = c\hbar k\phi$, $k > 0$. The momentum distribution $|\phi(k,t)|^2 = |g(k)|^2$ is non-zero only for $k > 0$ and remains constant in time. Also the position distribution $|\psi(x,t)|^2 = |f(x-ct)|^2$, moves with the speed c of light in the positive x direction and maintains its form. Since f is the Fourier transform of g , the uncertainty relation holds for the spread Δx and Δk namely $\Delta x \Delta k \ge \frac{1}{2}$, however both Δx and Δk are constant in time, there is no "time of minimum spread". Let $x_0 = \int_{-\infty}^{\infty} y|f(y)|^2\, dy$. Then

$$\langle x\rangle_t = \int_{-\infty}^{\infty} \psi^*(x,t)\, x\, \psi(x,t)\, dx = \int_{-\infty}^{\infty} x|f(x-ct)|^2\, dx$$

$$= \int_{-\infty}^{\infty} (y+ct)\, |f(y)|^2\, dy = x_0 + ct \ .$$

We assume f (and hence g) is normalized. Here $x_0 = \langle x\rangle_0$. This shows the centre of expectation in position space moves with the speed of light increasing with time.

Let us consider the normalized energy eigenfunctions $\psi_{\omega,x_1}(x)$. Since $H\psi_\omega(x) = \hbar\omega\psi_\omega(x)$ we obtain $-i\hbar c \frac{\partial}{\partial x} \psi_\omega(x) = \hbar\omega\psi_\omega(x)$ and so $\psi_\omega(x) = \lambda(\omega)\, e^{i\frac{\omega x}{c}}$. Normalization $\int_{-\infty}^{\infty} \psi^*_{\omega_1}(x)\psi_{\omega_2}(x)\, dx = \delta(\omega_1-\omega_2)$ implies that $|\lambda(\omega)| = \frac{1}{\sqrt{2\pi c}}$. Phasing $\psi_\omega(x)$ at $x = x_1$ we get $\psi_{\omega,x_1}(x) = \frac{1}{\sqrt{2\pi c}}\, e^{i\frac{\omega}{c}(x-x_1)}$. $\psi(x,t)$ is then expanded as

$$\psi(x,t) = \int_0^\infty A(\omega,x_1)\psi_{\omega,x_1}(x)\, e^{-i\omega t}\, d\omega \ .$$

Recall that $\omega = ck$. Substituting for $\psi_{\omega,x_1}(x)$ we get

$$\psi(x,t) = \frac{1}{\sqrt{2\pi c}} \int_0^\infty A(\omega,x_1)\, e^{i\frac{\omega}{c}(x-x_1)-i\omega t}\, d\omega \ .$$

Change variable in the integration to k from ω to get

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_0^\infty (\sqrt{c}\, A(ck,x_1)e^{-ikx_1})\, e^{ik(x-ct)}\, dk \ .$$

Comparison gives $g(k) = \sqrt{c}\, A(ck,x_1)\, e^{-ikx_1}$, so $A(\omega,x_1) = \frac{1}{\sqrt{c}}\, g(\frac{\omega}{c})\, e^{i\frac{\omega}{c}x_1}$. Clearly $A(\omega,x_1) = 0$ for $\omega \leq 0$. The time amplitude function $T(t,x_1)$ can be obtained by Fourier transforming $A(\omega, x_1)$ as

$$T(t,x_1) = \frac{1}{\sqrt{2\pi}} \int_0^\infty A(\omega,x_1)\, e^{-i\omega t}\, d\omega \ .$$

From this we have $T(t,x_1) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \sqrt{c}\, g(k)\, e^{ik(x_1-ct)}\, dk = \sqrt{c}\,\Psi(x_1,t)$,

$T(t,x_1) = \sqrt{c}\, f(x_1-ct)$. The relation between the time amplitude function and position wavefunction is $T(t,x) = \sqrt{c}\,\psi(x,t)$. Let us evaluate the expected time of arrival at x_1 . This is given by

$$\langle t\rangle_{x_1} = \int_{-\infty}^{\infty} t \,|T(t,x_1)|^2 dt = \int_{-\infty}^{\infty} tc \,|f(x_1-ct)|^2 \,dt \quad .$$

Let $y = x_1-ct$ so $dy = -cdt$ in the integral. Then

$$\langle t\rangle_{x_1} = \int_{\infty}^{-\infty} (x_1-y)\ |f(y)|^2 (-\frac{dy}{c}) = \frac{1}{c}\int_{-\infty}^{\infty} (x_1-y)\ |f(y)|^2\, dy$$

$$= \frac{1}{c}\,(x_1-x_0) \quad .$$

Thus the exected time of arrival at x_1 is $\frac{1}{c}\,(x_1-x_0)$. Recall $x_0 = \langle x\rangle_{t=0}$ and we see $\langle t\rangle_{x=x_0} = 0$.

CHAPTER VI

SCATTERING THEORY IN ONE DIMENSION

We have considered the wave function of a free particle in one dimension. Now, let us consider a potential $V(x)$ which is localized about $x = 0$. We assume $V(x) = 0$ for $|x| > a$.

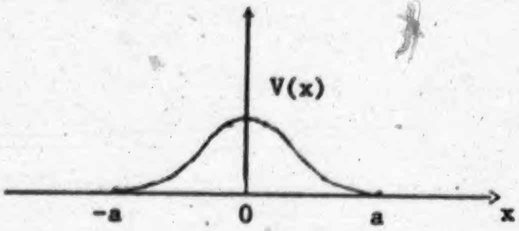

Figure 11

Local Potential

We then consider the Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = - \frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x) \quad .$$

In scattering theory, a basic assumption is made about the position wavefunction $\psi(x,t)$. We define the interaction probability of the particle with the potential at time t to be

$$p(t) = \int_{-a}^{a} |\psi(x,t)|^2 \, dx \quad .$$

We assume that $\psi(x,t)$ is such that $p(t)$ tends to zero (or is essentially zero) for t outside of an interval which is the time interval of interaction with the potential.

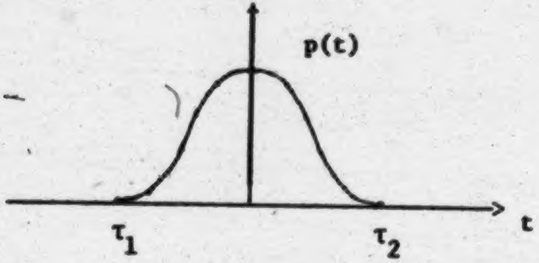

Figure 12

Time Interaction Interval

In otherwords, the particle does not react with the potential before and after scattering, and the solution for the wavefunction is the free particle solution. The momentum wavefunction before scattering is

$$\phi_1(k,t) = \phi_1(k,t_0)\, e^{-\frac{i\hbar k^2(t-t_0)}{2M}} ,$$

and after scattering it is

$$\phi_2(k,t) = \phi_2(k,t_0)\, e^{-\frac{i\hbar k^2(t-t_0)}{2M}} .$$

ϕ_1 is the wavefunction of the particle for $t < \tau_1$ and ϕ_2 is the momentum wavefunction for $t > \tau_2$. Each has the free particle time dependence. ϕ_2 is determined from ϕ_1 by the momentum transformation kernel $B_{t_0}(k,k')$ satisfying

$$\phi_2(k,t_0) = \int_{-\infty}^{\infty} B_{t_0}(k,k')\phi_1(k',t_0)dk' \tag{1}$$

for all t_0 . One can see that ϕ_2 depends linearly on ϕ_1 , since ϕ_1 and ϕ_2 are respectively the asymptotic solutions for ϕ at $t = -\infty$ and $+\infty$ respectively where ϕ satisfies the linear Schrödinger equation

$$i\hbar \frac{\partial\phi}{\partial t} = \frac{\hbar^2 k^2}{2M}\phi + V(i\frac{\partial}{\partial k})\phi$$

which is linear, although the operator $V(i\frac{\partial}{\partial k})$ makes it difficult to solve. Alternatively, ϕ is the Fourier transform of ψ satisfying

$$i\hbar \frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2M}\frac{\partial^2\psi}{\partial x^2} + V(x)\,\psi\ .$$

Specifying initial conditions ϕ_1 for ϕ determines ϕ for all time, and hence determines ϕ_2 . Moreover this dependence on ϕ_1 is linear, and so ϕ_2 depends on ϕ_1 . This justifies the form (1) of the transformation shown above. Moreover we can see that the kernel $B_{t_0}(k,k')$, like the Fourier transform kernel $\frac{1}{\sqrt{2\pi}}e^{ikx}$ preserves norm on the transformed wave-functions, since if we assume ϕ_1 is normalized, then ϕ_2 must be normalized also (for ϕ_1 a wave packet in momentum space).

Let us consider the dependence of $B_t(k,k')$ on t . We have $\phi_2(k,t) = \int_{-\infty}^{\infty} B_t(k,k')\ \phi_1(k',t)\ dk'$, so

$$\phi_2(k,t_0)\, e^{-\frac{i\hbar k^2(t-t_0)}{2M}} = \int_{-\infty}^{\infty} B_t(k,k')\phi_1(k',t_0)\, e^{-\frac{i\hbar k'^2(t-t_0)}{2M}}\, dk'$$

$$= e^{-\frac{i\hbar k^2(t-t_0)}{2M}} \int_{-\infty}^{\infty} B_{t_0}(k,k')\phi_1(k',t_0)\, dk' \quad .$$

Hence

$$B_t(k,k')\, e^{-\frac{i\hbar k'^2(t-t_0)}{2M}} = B_{t_0}(k,k')\, e^{-\frac{i\hbar k^2(t-t_0)}{2M}} \quad .$$

Thus we have

$$B_t(k,k') = B_{t_0}(k,k')\, e^{-\frac{i\hbar(k^2-k'^2)(t-t_0)}{2M}} \tag{2}$$

as the time dependence of the momentum transformation kernel.

Similarly, if we take Fourier transforms of ϕ_1 and ϕ_2 we can define ψ_1 and ψ_2 by

$$\psi_i(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi_i(k,t)\, e^{ikx}\, dk \quad \text{for} \quad i = 1,2,$$

and the position transformation kernel $A_t(x,x')$ by

$$\psi_2(x,t) = \int_{-\infty}^{\infty} A_t(x,x')\psi_1(x',t)\, dx' \quad . \tag{3}$$

Using (3) we can derive the relation between the position and momentum transformation kernels.

$$\phi_2(k,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \psi_2(x,t)e^{-ikx}dx = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} A_t(x,t')\psi_1(x',t)e^{-ikx}dxdx' \;.$$

We now substitute $\psi_1(x',t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \phi_1(k',t)e^{ik'x'}dk'$ to get

$$\phi_2(k,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} A_t(x,x')e^{-ikx}e^{ik'x'}\,\phi_1(k',t)dxdx'dk'$$

$$= \int_{-\infty}^{\infty} B_t(k,k')\,\phi_1(k',t)\,dk' \;.$$

Hence

$$B_t(k,k') = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} A_t(x,x')e^{-ikx}e^{ik'x'}dxdx' \;. \tag{4}$$

Similarly, the inverse relation is given by

$$A_t(x,x') = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} B_t(k,k')e^{ikx}e^{-ik'x'}dkdk' \;. \tag{5}$$

From (5) and (2) the time dependence of $A_t(x,x')$ can be determined.

We define the time shift operator in position space by $T_{(t-t_0)}\psi(x,t_0) = \psi(x,t)$, where T operates on functions of x and is norm preserving. Since

$$\psi(x,t) = \frac{(1-i)}{2}\sqrt{\frac{M}{\pi\hbar(t-t_0)}}\int_{-\infty}^{\infty} \psi(\bar{x},t_0)\,\exp\left(\frac{iM(x-\bar{x})^2}{2\hbar(t-t_0)}\right)\,d\bar{x} \;,$$

the kernel $T(x,\bar{x})$ defining the time shift operator, with

$$\psi(x,t) = \int_{-\infty}^{\infty} T_{(t-t_0)}(x,\bar{x})\, \psi(\bar{x},t_0)\, dx$$

is given by

$$T_{(t-t_0)}(x,\bar{x}) = \frac{1-i}{2}\sqrt{\frac{M}{\pi\hbar(t-t_0)}}\, \exp\left(\frac{iM(x-\bar{x})^2}{2\hbar(t-t_0)}\right) \quad . \qquad (6)$$

The time shift operator composes in time, i.e. $T_{t_1} \circ T_{t_2} = T_{t_1+t_2}$. This can be seen since $T_{t_1} \circ T_{t_2} \psi(x,0) = \psi(x,t_1+t_2) = T_{t_1+t_2}\, \psi(x,0)$ for arbitrary $\psi(x,0)$. The inverse of T_t is T_{-t} and T_0 is the identity operator and has the kernel $T_0(x,\bar{x}) = \delta(x-\bar{x})$. Note that

$$T_t\, e^{ikx} = e^{(ikx - \frac{i\hbar k^2 t}{2M})} \quad . \qquad (7)$$

This means e^{ikx} is an eigenfunction of T_t with eigenvalue $e^{-\frac{i\hbar k^2 t}{2M}}$.

Let us use the time shift operator in position space to determine the time dependence of the position transformation kernel. We observe that $\psi_2(x,t) = \int_{-\infty}^{\infty} A_t(x,x')\, \psi_1(x',t)\, dx'$, and

$$\psi_2(\bar{x},t_0) = \int_{-\infty}^{\infty} A_{t_0}(\bar{x},x')\, \psi_1(x',t_0)\, dx' \ .$$

Also

$$\psi_2(x,t) = \int_{-\infty}^{\infty} T_{(t-t_0)}(x,\bar{x})\psi_2(\bar{x},t_0)\, d\bar{x}$$

and $\psi_1(x',t_0) = \int_{-\infty}^{\infty} T_{(t_0-t)}(x',\bar{\bar{x}})\psi_1(\bar{\bar{x}},t)d\bar{\bar{x}}$. Thus we have that

$$\psi_2(x,t) = \int_{-\infty}^{\infty} T_{(t-t_0)}(x,\bar{x})\ \psi_2(\bar{x},t_0)\ d\bar{x}$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} T_{(t-t_0)}(x,\bar{x})A_{t_0}(\bar{x},x')\ \psi_1(x',t_0)dx'd\bar{x}$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} T_{(t-t_0)}(x,\bar{x})A_{t_0}(\bar{x},x')T_{(t_0-t)}(x',\bar{\bar{x}})\psi_1(\bar{\bar{x}},t) \times d\bar{\bar{x}}dx'd\bar{x}$$

$$= \int_{-\infty}^{\infty} A_t(x,\bar{\bar{x}})\ \psi_1(\bar{\bar{x}},t)\ d\bar{\bar{x}} \quad .$$

This implies

$$A_t(x,\bar{\bar{x}}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} T_{(t-t_0)}(x,\bar{x})\ A_{t_0}(\bar{x},x')T_{(t_0-t)}(x',\bar{\bar{x}})dx'd\bar{x} \qquad (8)$$

is the time dependence of the position transformation operator.

In operator notation, equation (8) reads as

$$A_t = T_{(t-t_0)}\ A_{t_0} T_{t_0-t} \quad .$$

The Delta Function Potential

Let us consider the simple potential $V(x) = V_0\ \delta(x)$, and determine the position and momentum transformation kernels.

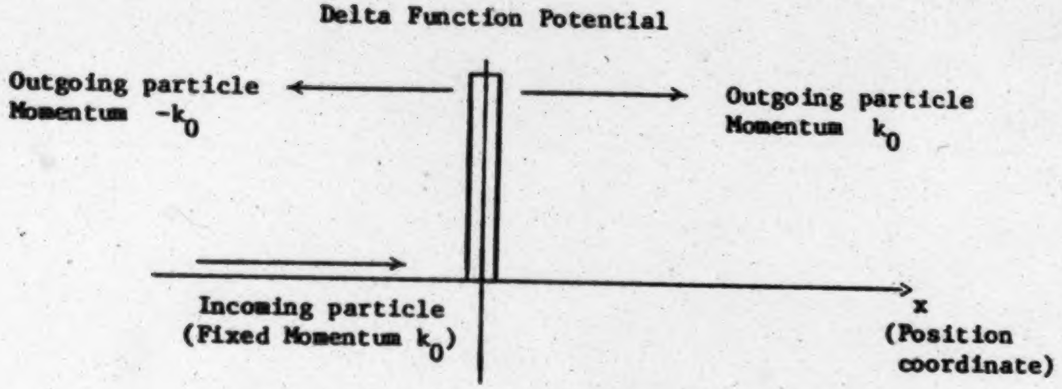
Delta Function Potential
Outgoing particle
Momentum $-k_0$
Outgoing particle
Momentum k_0
Incoming particle
(Fixed Momentum k_0)
x
(Position
coordinate)

Figure 13

Delta Function Potential

Let us take the initial momentum wavefunction for large negative t to be $\phi_1(k,t) = \delta(k-k_0)e^{-i\omega t}$ where $\omega = \frac{hk_0^2}{2M}$. In practice, we must take a superposition over a finite interval of k and not a discrete value, in order to normalize and satisfy the condition of zero interaction with the potential at distant future and past times. However this simple method allows us to get results easily.

We assume the standard scattering phenomenom, namely no interaction with the potential, followed by interaction with the potential followed by no interaction. (The k-width is finite but extremely narrow.) Hence we can assert that the initial particle momentum is k_0 and energy is $\frac{\hbar^2 k_0^2}{2M}$. But the scattering is elastic, and so the final energy is also $\frac{\hbar^2 k_0^2}{2M}$ after interaction with the potential is complete. This means the final momentum is either $+k_0$ or $-k_0$ with relative probabilities to be determined.

Hence the final momentum wavefunction for large positive time t is $\phi_2(k,t) = [\alpha\delta(k-k_0) + \beta\delta(k+k_0)]\, e^{-i\omega t}$ where α and β are unknown complex constants and ω is the constant $\omega = \frac{\hbar k_0^2}{2M}$.

Let us see what can be done about determining α and β . First of all, we determine the corresponding position wavefunction by Fourier transforming. Thus

$$\psi_1(x,t) = \frac{1}{\sqrt{2\pi}}\, e^{ik_0 x}\, e^{-i\omega t} \quad ,$$

$$\psi_2(x,t) = \frac{1}{\sqrt{2\pi}}\, [\alpha e^{ik_0 x} + \beta e^{-ik_0 x}]\, e^{-i\omega t} \quad .$$

Consider now the position wavefunction $\psi(x,t)$ satisfying the equation

$$i\hbar \frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2M} \frac{\partial^2\psi(x,t)}{\partial x^2} + V_0\, \delta(x)\, \psi(x,t) \quad .$$

We know that for $x < 0$ ψ is a superposition, and for $x > 0$, a single wave. Thus we take

$$\psi(x,t) = (A\, e^{ik_0 x} + B\, e^{-ik_0 x})\, e^{-i\omega t} \quad \text{for} \quad x < 0 \quad ,$$

$$\psi(x,t) = C\, e^{ik_0 x}\, e^{-i\omega t} \quad \text{for} \quad x > 0 \quad .$$

We must satisfy boundary conditions at $x = 0$ namely $\psi(0^+,t) = \psi(0^-,t)$ and $\frac{\partial\psi}{\partial x}(0^+,t) - \frac{\partial\psi}{\partial x}(0^-,t) = \frac{2mV_0}{\hbar^2}\, \psi(0,t)$. Hence

$C\,e^{-i\omega t} = (A+B)e^{-i\omega t} = \psi(0,t)$ so $A+B = C$, and,

$$ik_0 Ce^{-i\omega t} - (Aik_0 - Bik_0)e^{-i\omega t} = \frac{2mV_0}{\hbar^2}\,C\,e^{-i\omega t}$$

or

$$ik_0 C - ik_0 A + ik_0 B = \frac{2mV_0 C}{\hbar^2} \quad .$$

One of these constants A is arbitrary (the multiplicative factor for the whole wave function) and so we may take $A = \frac{1}{\sqrt{2\pi}}$. Doing this we get

$ik_0(\frac{1}{\sqrt{2\pi}} + B) - ik_0 \frac{1}{\sqrt{2\pi}} + ik_0 B = \frac{2mV_0}{\hbar^2}(\frac{1}{\sqrt{2\pi}} + B)$, so that

$$\sqrt{2\pi}\,B = \frac{mV_0}{ik_0\hbar^2 - mV_0} \quad \text{and} \quad \sqrt{2\pi}\,C = \frac{ik_0\hbar^2}{ik_0\hbar^2 - mV_0} \quad .$$

This determines the wavefunction $\psi(x,t)$ as

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\left(e^{ik_0 x} + \frac{mV_0}{ik_0\hbar^2 - mV_0}e^{-ik_0 x}\right)e^{-i\omega t} \qquad \text{for } x < 0 \ ,$$

$$= \frac{1}{\sqrt{2\pi}}\,\frac{ik_0\hbar^2}{ik_0\hbar^2 - mV_0}\,e^{ik_0 x}\,e^{-i\omega t} \qquad \text{for } x > 0 \ .$$

Comparing with initial and final conditions for $\psi_1(x,t)$ and $\psi_2(x,t)$ we see that $\frac{\alpha}{\sqrt{2\pi}} = C = \frac{1}{\sqrt{2\pi}}\,\frac{ik_0\hbar^2}{ik_0\hbar^2 - mV_0}$. Also $\frac{\beta}{\sqrt{2\pi}} = B = \frac{1}{\sqrt{2\pi}}\,\frac{mV_0}{ik_0\hbar^2 - mV_0}$.

Thus we determine the final momentum wavefunction as

$$\phi_2(k,t) = [\frac{ik_0\hbar^2}{ik_0\hbar^2 - mV_0}\,\delta(k-k_0) + \frac{mV_0}{ik_0\hbar^2 - mV_0}\,\delta(k+k_0)]\ e^{-i\omega t} .$$

This was transformed from the initial momentum wavefunction, namely $\phi_1(k,t) = \delta(k-k_0)\ e^{-i\omega t}$. But we know $\phi_2(k,t) = \int_{-\infty}^{\infty} B_t(k,k')\phi_1(k',t)\ dk'$ and so we can determine $B_t(k,k')$. $\phi_2(k,t) = \int_{-\infty}^{\infty} B_t(k,k')\ \delta(k'-k_0)e^{-i\omega t}dk' = B_t(k,k_0)\ e^{-i\omega t}$. Thus

$$B_t(k,k_0) = \frac{ik_0\hbar^2}{ik_0\hbar^2 - mV_0}\,\delta(k-k_0) + \frac{mV_0}{ik_0\hbar^2 - mV_0}\,\delta(k+k_0) \qquad (9)$$

is the momentum transformation kernel. Observe that it does not depend on t . We have seen that the time dependence of the momentum transformation kernel in general is given by (2) namely

$$B_t(k,k') = B_{t_0}(k,k')\ e^{-\frac{i\hbar(k^2-k'^2)(t-t_0)}{2M}} .$$

We observe that from (9) for the case of a δ potential in 1 dimension, $B_{t_0}(k,k') = 0$ if $k^2 \neq k'^2$ and so the time dependent term is simply 1 and $B_t(k,k')$ does not depend on t .

Let us consider the relative probability of transmission or reflection. A normalized wave packet of very narrow momentum width about k_0 interacts with the potential $V_0\ \delta(x)$ and two wave packets result; one of narrow width about k_0 and one of narrow width about $-k_0$. The integral of the absolute value squared of the wave function over the small interval in momentum space for each case determines the probability. For discrete k_0 we see that the probability of transmission is $\frac{k_0^2 \hbar^4}{k_0^2\hbar^4 + m^2V_0^2}$ and the probability of reflection is $\frac{m^2 V_0^2}{k_0^2\hbar^4 + m^2V_0^2}$.

Potentials of Finite Width

Let $V(x)$ be a potential (usually positive) that is zero outside the interval $-a \leq x \leq a$. The strength of the potential is $\int_{-a}^{a} V(x)\,dx$. This is essentially a product of magnitude and range. We assume the potential is positive and does not change sign.

The delta function potential gives a good approximation to the momentum transformation if the deBroglie wavelength of the incoming particle is much greater than the range $2a$ of the potential. In this case one can determine the strength V_0 of the potential, by measuring the transmission reflection probabilities for particles of known mass M and momentum $\hbar k_0$.

Let us consider the finite width potential, and for simplicity take it to be constant on this range. Let the magnitude be E_0 and the range $2a$ so that the strength is $V_0 = 2a\ E_0$.

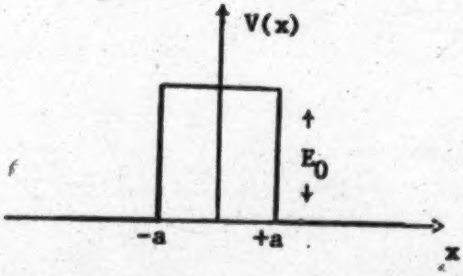

Figure 14

Square Potential Barrier

We can do the same type of calculation in this case, assuming an initial and final momentum wavefunction of exactly the same form as in the case of the delta function potential. We can solve the time independent Schrödinger equation in this case, because we know that the time dependence is $e^{-i\omega t}$ where $\omega = \frac{\hbar k_0^2}{2M}$. Thus

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\,\psi(x) = \frac{\hbar^2 k_0^2}{2m}\psi(x) .$$

We have the general form for $\psi(x)$ when $x < -a$ and $x > a$ as

$$\psi(x) = \begin{cases} (Ae^{ik_0x} + Be^{-ik_0x}) & \text{for } x < -a \\ C\,e^{ik_0x} & \text{for } x > a . \end{cases}$$

Now we solve for $\psi(x)$ on $-a \leq x \leq a$ in such a way that ψ and its derivative are both continuous at $|x| = a$. On this interval, the differential equation satisfied is $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = (\frac{\hbar^2 k_0^2}{2m} - E_0)\,\psi(x)$ or $\frac{d^2\psi}{dx^2} + (k_0^2 - \frac{2mE_0}{\hbar^2})\,\psi(x) = 0$. The solution is

$$\psi(x) = D\exp(i\sqrt{k_0^2 - \frac{2mE_0}{\hbar^2}}\,x) + E\exp(-i\sqrt{k_0^2 - \frac{2mE_0}{\hbar^2}}\,x)$$

where the square root is a positive multiple of 1 or i depending on the sign of $k_0^2 - \frac{2mE_0}{\hbar^2}$. As before, one of the coefficients is arbitrary, and we may take $A = \frac{1}{\sqrt{2\pi}}$ in order to uniquely determine B , C , D , E .

Let $\lambda = \sqrt{k_0^2 - \frac{2mE_0}{\hbar^2}}$. We have

$$E = \frac{2k_0(\lambda-k_0)e^{i(\lambda-k_0)a}}{\sqrt{2\pi}\ S} , \quad D = \frac{2k_0(\lambda+k_0)e^{-i(\lambda+k_0)a}}{\sqrt{2\pi}\ S} \tag{10}$$

$$C = \frac{4k_0\lambda e^{-2ik_0a}}{\sqrt{2\pi}\ S} , \quad B = \frac{2k_0[(\lambda-k_0)e^{2i(\lambda-k_0)a} + (\lambda+k_0)e^{-2i(\lambda+k_0)a}]}{\sqrt{2\pi}\ S} - \frac{e^{-2ik_0a}}{\sqrt{2\pi}}$$

where $S = (k_0+\lambda)^2 e^{-2i\lambda a} - (\lambda-k_0)^2 e^{2i\lambda a}$.

These are the explicit solutions for the coefficients of the position wavefunction. Because of their awkwardness, we shall simply use the symbols B , C , D , E and λ rather than the explicit expressions given in (10) above which are listed for reference.

We have the wavefunction $\psi(x)$ given by

$$\begin{aligned} \psi(x) &= \frac{e^{ik_0x}}{\sqrt{2\pi}} + Be^{-ik_0x} && \text{for} \quad x < -a \\ &= D\,e^{i\lambda x} + E\,e^{-i\lambda x} && \text{for} \quad -a < x < a \\ &= C\,e^{ik_0x} && \text{for} \quad x > a \end{aligned} \tag{11}$$

where B , C , D , E and λ are defined in (10). As in the case of the delta function potential, the wavefunction ψ_1 before scattering and ψ_2 after scattering are

$$\psi_1(x) = \frac{e^{ik_0x}}{\sqrt{2\pi}} \quad , \quad \psi_2(x) = Be^{-ik_0x} + Ce^{ik_0x} \quad .$$

For $\omega = \frac{\hbar k_0^2}{2m}$ the time dependence of ψ_1 and ψ_2 gives us

$$\psi_1(x,t) = \frac{e^{ik_0x-i\omega t}}{\sqrt{2\pi}} \quad , \quad \psi_2(x,t) = (Be^{-ik_0x} + Ce^{ik_0x})\, e^{-i\omega t} \quad .$$

By Fourier transforming we obtain the intial and final momentum wavefunction as

$$\phi_i(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi_i(x,t)\, e^{-ikx}\, dx \qquad \text{for } i = 1,2$$

$$\phi_1(k,t) = \delta(k_0-k)\, e^{-i\omega t}$$

$$\phi_2(k,t) = \sqrt{2\pi}\, [C\, \delta(k_0-k) + B\delta(k_0+k)]\, e^{-i\omega t} \quad .$$

From this we can determine the momentum transformation kernel as

$$B_t(k,k_0) = \sqrt{2\pi}\, [C\delta(k_0-k) + B\delta(k_0+k)] \tag{12}$$

A very important result in one dimensional scattering theory from local potentials is the generality of equation (12) for the momentum transformation kernel in the case of elastic (potential) interactions. The coefficients C and D are functions of k_0 which depend on the nature of the potential V(x) .

If the potential $V(x)$ is local, so that $V(x) = 0$ for $x < -a$ and $x > a$, the free particle equation is satisfied, and so the positive momentum solution takes the form

$$\psi(x) = \begin{cases} \dfrac{e^{ik_0x}}{\sqrt{2\pi}} + B\,e^{-ik_0x} & \text{for} \quad x < -a \\ \\ C\,e^{ik_0x} & \text{for} \quad x > a \quad . \end{cases}$$

ψ has a behaviour depending on $V(x)$ for $-a < x < a$, but B and C can be determined for given $V(x)$ by matching values and derivatives of ψ at $-a$ and a. Once B and C are found, the momentum transformation kernel is given by

$$B_t(k,k_0) = \sqrt{2\pi}\,[C\delta(k_0-k) + B\delta(k_0+k)] \quad ,$$

where C and B depend on k_0 and $B_t(k,k_0)$ is independent of t.

Probabilities of Reflection and Transmission

For incident particles (or wave packets) of momentum k_0, the probability of reflection is $2\pi|B|^2$ and the probability of transmission is $2\pi|C|^2$. This implies $2\pi(|C|^2 + |B|^2) = 1$. Observe that C and B are functions of k_0. For the finite range potential described earlier, (see equations (10))

$$T = 2\pi|C|^2 = \frac{16\ k_0^2\ |\lambda|^2}{|S|^2} \ .$$

In the case where λ is real and positive we have

$$T = \frac{16\ k_0^2\ \lambda^2}{(k_0+\lambda)^4 + (k_0-\lambda)^4 - 2(\lambda-k_0)^2(\lambda+k_0)^2 \cos(4\lambda a)} \ .$$

This puts bounds on T , namely

$$1 \geq T \geq \left(\frac{2k_0\lambda}{k_0^2 + \lambda^2}\right)^2 \ ,$$

by considering the limits on $\cos(4\lambda a)$. If $\lambda = i|\lambda|$ (λ is imaginary), T can be expressed as

$$T = \frac{8\ k_0^2\ |\lambda|^2}{4|\lambda|^2k_0^2 - (|\lambda|^2-k_0^2)^2 + (k_0^2+|\lambda|^2)^2 \cosh(4|\lambda|a)} \ .$$

The transmission coefficient T can be measured as a function of k_0 . In the case of the square potential, it provides a means for obtaining the parameters E_0 and a . For the general potential, it gives us the absolute value of the functions C and B of k_0 . It does not give us any information about the phase, and consequently the momentum transformation kernel is not completely determined. We might ask if time delay measurements can provide this phase information.

Time Delay: Its Relation to the Momentum Transformation Kernel.

Suppose that the initial wave packet before interaction is described by the momentum wavefunction $\phi_1(k,t)$ with the free particle time dependence $\phi_1(k,t) = \phi_1(k,t_0)\, e^{-i\hbar k^2(t-t_0)/2M}$. Let us suppose that ϕ_1 has a localized positive momentum distribution about $k_0 > 0$, and ϕ_1 is zero for all k less than some fixed k_1 with $0 < k_1 < k_0$. This wave packet interacts with the potential, is scattered, and the resulting free particle wave function is $\phi_2(k,t)$. For a momentum transformation kernel given by

$$B_t(k,k') = \sqrt{2\pi}\,[C(k')\delta(k'-k) + B(k')\delta(k'+k)]$$

the resulting $\phi_2(k,t)$ is

$$\phi_2(k,t) = \sqrt{2\pi}\,C(k)\phi_1(k,t) + \sqrt{2\pi}\,B(-k)\phi_1(-k,t) \quad .$$

Because $\phi_1(k,t)$ is non-zero only for positive k,

$$\phi_2(k,t) = \begin{cases} \sqrt{2\pi}\,C(k)\,\phi_1(k,t) & \text{for} \quad k > 0 \\ \sqrt{2\pi}\,B(-k)\phi_1(-k,t) & \text{for} \quad k < 0 \quad . \end{cases}$$

If we graph $|\phi_2(k,t)|^2$ as a function of k, we can see that there are two distributions; one about k_0 and one about $-k_0$.

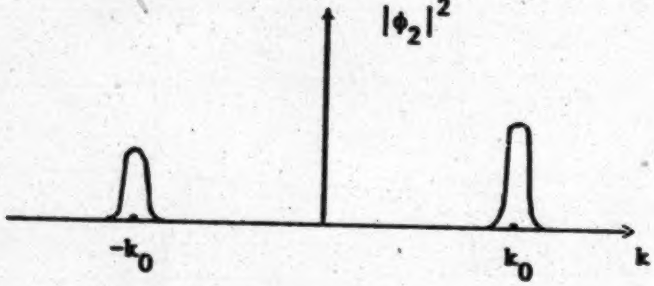

Figure 15

Momentum Distribution
After Scattering

Determining the Potential $V(x)$ From the Momentum Transformation Kernel.

The WKB Approximation. Suppose that the initial energy level $\frac{1}{2}mV_0^2$ is large compared to the maximum height of the potential over the range of the narrow momentum wavepacket centred at $k_0 = \frac{mV_0}{\hbar}$. Suppose also that the potential is smooth and slowly varying over the range of one wavelength $\lambda = \frac{2\pi}{k_0}$.

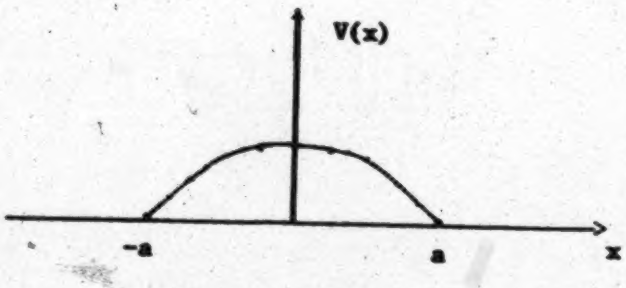

Figure 16

Slowly Varying Potential

We use the WKB approximation to represent the solution $\psi(x)$ to the Schrödinger equation in terms of the potential $V(x)$. We match this solution for $-a < x < a$ to the exterior solution

$$\psi(x) = \begin{cases} \dfrac{e^{ik_0x}}{\sqrt{2\pi}} + B\, e^{-ik_0x} & \text{for} \quad x < -a \quad , \\ \\ C\, e^{ik_0x} & \text{for} \quad x > a \quad . \end{cases}$$

From this we can express B and C in terms of the potential $V(x)$.

The solution for ψ on $-a$ to a is given approximately by

$$\psi^{\pm}(x) = \psi^{\pm}(x_0) \sqrt[4]{\frac{\hbar^2 k_0^2 - 2mV(x_0)}{\hbar^2 k_0^2 - 2mV(x)}} \; \exp[\pm i \int_{x_0}^{x} \sqrt{k_0^2 - \frac{2m}{\hbar^2} V(x)}\; dx] \quad .$$

We assume that $V(x)$ is smooth and that V and its first derivative are zero at $\pm a$. The interior solution is assumed to be

$$\psi(x) = D\psi^{+}(x) + E\psi^{-}(x) \quad \text{for} \quad -a < x < a \quad .$$

Let us take $\psi^{+}(-a) = \psi^{-}(-a) = 1$. From this we get that

$$\psi^{\pm}(a) = \exp[\pm i \int_{-a}^{a} \sqrt{k_0^2 - \frac{2m}{\hbar^2} V(x)}\; dx] \quad \text{and} \quad \psi^{\pm}(-a) = 1 \quad ;$$

$$\frac{d}{dx}\psi^{\pm}(a) = \pm ik_0 \exp[\pm i \int_{-a}^{a} \sqrt{k_0^2 - \frac{2m}{\hbar^2} V(x)}\; dx] \quad ,$$

and $\frac{d}{dx}\psi^{\pm}(-a) = \pm ik_0$.

For simplicity, let us define $\gamma(k_0)$ by

$$\gamma(k_0) = \int_{-a}^{a} \sqrt{k_0^2 - \frac{2m}{\hbar^2} V(x)}\ dx = \gamma \ .$$

Continuity of ψ and its derivatives at $\pm a$ give us the equations

$$C e^{ik_0a} = D e^{i\gamma} + E e^{-i\gamma}$$

$$\frac{e^{-ik_0a}}{\sqrt{2\pi}} + B e^{ik_0a} = D + E$$

$$C e^{ik_0a} = D e^{i\gamma} - E e^{-i\gamma}$$

$$\frac{e^{-ik_0a}}{\sqrt{2\pi}} - B e^{ik_0a} = D - E \ .$$

These very simple equations tell us that $E = 0$ and $D = \frac{e^{-ik_0a}}{\sqrt{2\pi}}$. Also we get $B = 0$ and $C = \frac{e^{i\gamma - 2ik_0a}}{\sqrt{2\pi}}$. Thus in this crude high energy approximation, there is no reflection, and only transmission. In this case it is not the reflection, and transmission coefficients which provide us with a direct link to the potential $V(x)$, but rather the phase of the transmission coefficient C that satisfies $|C|^2 = \frac{1}{2\pi}$.

The momentum transformation kernel turns out to be

$B_t(k,k_0) = e^{i\gamma(k_0) - 2ik_0a}\,\delta(k_0-k)$, and hence

$$\phi_2(k,t) = \phi_1(k,t)\ e^{i\gamma(k)-2ika} \quad . \tag{13}$$

ϕ_2 has the same momentum distribution as ϕ_1 . Consequently measurements which are designed to determine $\gamma(k)$ as a function of k must involve position or time delay. Observe that (13) is a good approximation for high energy, and yet from it we can determine the potential $V(x)$ which can be used in lower energy exact calculations to explicitly obtain the momentum transformation kernel.

We note that both ϕ_2 and ϕ_1 have positive momentum distributions. Consequently, we can apply the free particle time operator as we have derived it in order to make time delay measurements.

Let us look at $\gamma(k) - 2ka$ in the term $\exp\{i(\gamma(k)-2ka)\}$

$$\gamma(k) - 2ka = \int_{-a}^{a} \sqrt{k^2 - \frac{2m}{\hbar^2} V(x)}\ dx - 2ka$$

$$= -\frac{m}{\hbar^2 k} V_1 - \sum_{n=1}^{\infty} \frac{(2n-1)!\,m^{n+1}\ V_{n+1}}{2^{n-1}(n-1)!\,(n+1)!\,\hbar^{2n+2} k^{2n+1}} \quad ,$$

where

$$V_n = \int_{-a}^{a} [V(x)]^n\ dx \quad .$$

We let

$$\lambda(k) = -\gamma(k) + 2ka$$

$$= \frac{mV_1}{\hbar^2 k} + \sum_{n=1}^{\infty} \frac{(2n-1)!\ m^{n+1}\ V_{n+1}}{2^{n-1}(n-1)!\,(n+1)!\,\hbar^{2n+2} k^{2n+1}}$$

so that $\phi_2(k,t) = \phi_1(k,t)\, e^{-i\lambda(k)}$.

Let us assume that ϕ_1 has a very narrow momentum distribution about $k_0 > 0$, and let us calculate $\langle t\rangle_{x_0}$ with respect to ϕ_1 and then ϕ_2 .

We know that $\langle t\rangle_{x_0} = \langle \tau_0\rangle_t$ on the momentum wavefunction where

$$\tau_0 = t - \frac{im}{\hbar k}\frac{\partial}{\partial k} + \frac{x_0 m}{\hbar k} + \frac{im}{2\hbar k^2} \quad .$$

Case 1: The Momentum Wavefunction ϕ_1 .

$$\langle \tau_0\rangle_t^{(1)} = t - \frac{\langle x\rangle_t^{(1)} m}{\hbar k_0} + \frac{x_0 m}{\hbar k_0} = t + (x_0 - \langle x\rangle_t^{(1)})\,\frac{m}{\hbar k_0} \quad ,$$

$$\langle x\rangle_t^1 = \int_0^\infty \phi_1^*(k,t)\left(i\,\frac{\partial}{\partial k}\right)\,\phi_1(k,t)\,dk.$$

Case 2: The Momentum Wavefunction ϕ_2 .

$$\langle \tau_0\rangle_t^{(2)} = t - \frac{\langle x\rangle_t^{(2)} m}{\hbar k_0} + \frac{x_0 m}{\hbar k_0} = t + (x_0 - \langle x\rangle_t^{(2)})\,\frac{m}{\hbar k_0}$$

$$\langle x\rangle_t^{(2)} = \int_0^\infty \phi_1^*(k,t)e^{i\lambda(k)}\left(i\,\frac{\partial}{\partial k}\right)\,[\phi_1(k,t)e^{-i\lambda(k)}]\,dk \quad .$$

For a time delay, we expect time of arrival to be later for ϕ_2 and so

$$\begin{aligned} \Delta t &= \langle\tau_0\rangle_t^{(2)} - \langle\tau_0\rangle_t^{(1)} \\ &= \left(\langle x\rangle_t^{(1)} - \langle x\rangle_t^{(2)}\right) \frac{m}{\hbar k_0} \\ &= -\frac{m}{\hbar k_0} \lambda'(k_0) \quad . \end{aligned}$$

Now taking the infinite series for $\lambda(k)$, differentiating and substituting we get

$$\Delta t = \sum_{n=1}^{\infty} \frac{(2n-1)!m^{n+1} V_n}{2^{n-1}(n-1)!n!\hbar^{2n+1}k_0^{2n+1}} \quad . \tag{14}$$

If we substitute $v_0 = \frac{\hbar k_0}{m}$ into (14) we get the classical time delay result

$$\Delta t = \sum_{n=1}^{\infty} \frac{(2n-1)! V_n}{(n-1)!n!2^{n-1}m^n v_0^{2n+1}} \quad .$$

The above calculations show that the classical time delay corresponds to the expected value of quantum mechanical time delay for high energy particles and slowly varying potentials.

CHAPTER VII

QUANTUM MECHANICAL TIME MEASUREMENT IN ONE DIMENSION

The measurement of time of arrival in quantum mechanics is limited by fundamental difficulties inherent in time measurements. Unlike position, momentum, energy or angular momentum, time is an improper and not not a proper quantum mechanical observable. This means that an operator associated with time measurements is not self-adjoint but only Hermitian. This means that time measurements cannot be made on every possible state of the system defined by a given Hamiltonian, but only on a restricted class of states defined by a subspace of the Hilbert space in question. The following free particle example illustrates this.

Consider the free particle in one dimension. Classically, the Hamiltonian is $H = \frac{p^2}{2m}$ independent of q. Thus $\frac{\partial H}{\partial p} = \frac{p}{m} = \dot{q}$ and $\frac{\partial H}{\partial q} = 0 = -\dot{p}$. The time function is $\tau_0(t,p,q) = t + \tau(p,q)$ where $\{H,\tau\} = 1$ where $\{\ \}$ is the Poisson bracket. This means that τ_0 like H is a constant of the motion. $\{H,\tau\} = 1 = \frac{\partial H}{\partial q}\frac{\partial \tau}{\partial p} - \frac{\partial H}{\partial p}\frac{\partial \tau}{\partial q} = -\frac{\partial \tau}{\partial q}\frac{p}{m}$. Thus $\frac{\partial \tau}{\partial q} = -\frac{m}{p}$ and $\frac{\partial \tau}{\partial p}$ is arbitrary. This means $\tau = -\frac{mq}{p} + f(p)$ for some (real) function $f(p)$ which is unknown. Quantum mechanically, we construct[1] the operator corresponding to τ_0 by

$$\tau_0(p,q,t) \rightarrow \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{i\hbar}{2}\right)^n \frac{\partial^{2n}\tau_0}{\partial q^n \partial p^n}$$

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[1] M. Razavy, Am. J. Phys. 35, 10(1967), p. 958

so that $\tau_0 \rightarrow +t - \frac{mq}{p} + f(p) + \frac{i\hbar}{2}\left(\frac{m}{p^2}\right)$ where the p factors appear before the q factors (i.e. operate first) in each term. Thus, as an operator,

$$\tau_0 = -t - \frac{m}{\hbar k}\left(i\frac{\partial}{\partial k}\right) + f(\hbar k) + \frac{im}{2\hbar k^2} \; .$$

In momentum space the time operator for a free particle in one dimension is

$$\tau_0 = t - \frac{im}{\hbar k}\frac{\partial}{\partial k} + f(\hbar k) + \frac{im}{2\hbar\, k^2} \; .$$

The unknown function (not determined here) turns out to be $f(\hbar k) = \frac{x_0 m}{\hbar k}$ where x_0 is the position at which time measurement is taken. Thus the time operator is

$$\tau_0 = t - \frac{im}{\hbar k}\frac{\partial}{\partial k} + \frac{x_0 m}{\hbar k} + \frac{im}{2\hbar k^2} \; .$$

This can be used to make time measurements. The expected time of arrival at x_0 is given by $\langle t\rangle_{x_0} = \langle\tau_0\rangle_t$ on the momentum wavefunction $\phi(k,t)$. For narrow positive momentum distributions about $k_0 > 0$ we can estimate $\langle\tau_0\rangle_t$ on the momentum wavefunction $\phi(k,t)$. It is

$$\langle\tau_0\rangle_t = t - \frac{m}{\hbar k_0}\langle x\rangle_t + \frac{x_0 m}{\hbar}\left\langle\frac{1}{k}\right\rangle_t \; .$$

This is a constant, independent of t and so $\frac{d}{dt}\langle x\rangle_t = \frac{\hbar k_0}{m} = v$ the velocity of propogation. The commutator of H and τ_0 is $[H,\tau_0] = i\hbar$

where $H = \frac{\hbar^2 k^2}{2m}$. This means that $\Delta\tau_0 \Delta H \geq \frac{\hbar}{2}$, the time-energy uncertainty relation.

The problem with τ_0 is the appearance of k and k^2 in the denominator in the terms $-\frac{im}{\hbar k} \frac{\partial}{\partial k}$ and $\frac{im}{2\hbar k^2}$. This imposes a restriction on the class of admissible momentum wavefunctions on which τ_0 can operate. (e.g. it excludes momentum distributions concentrated about $k = 0$.) This means that τ_0 is not self-adjoint, but only Hermitian. Its domain of operation is not the complete Hilbert space.

We can illustrate the statement that an operator conjugate to the Hamiltonian will not in general be self-adjoint but only Hermitian in the case of a Hamiltonian with discrete energy levels like that of the one dimensional Harmonic oscillator. For $H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m\omega^2 x^2$, the energy eigenfunctions are $\psi_n(x) = \sqrt{\beta}\, \pi_n(\beta x)$ where $H\psi_n(x) = (n + \frac{1}{2})\hbar\omega\psi_n(x)$ and $\beta = \sqrt{\frac{m\omega}{\hbar}}$ and $\pi_n(\gamma) = \frac{1}{\sqrt{2^n\, n!\sqrt{\pi}}} H_n(\gamma)\, e^{-\gamma^2/2}$. The infinite matrix representing H is diagonal $\{E_0, E_1, E_2, E_3, \cdots\}$ where $E_n = (n + \frac{1}{2})\hbar\omega$. The elements are denoted by $H_{mn} = \langle\psi_m|H|\psi_n\rangle = E_n\, \delta_{nm}$. What are the matrix elements of an operator τ conjugate to H ? They are $\tau_{mn} = \langle\psi_m|\tau|\psi_n\rangle$. If $[H,\tau] = i\hbar$ we require $H_{mn}\, \tau_{n\ell} - \tau_{mn}\, H_{n\ell} = i\hbar\, \delta_{m\ell}$. But $H_{mn} = E_n\, \delta_{nm}$ and so we get that $\tau_{m\ell} = \frac{i\hbar\delta_{m\ell}}{E_m - E_\ell}$, which indicates that the operator τ transforms a vector ψ_n of unit norm to one of infinite norm (i.e. out of the Hilbert space). Thus τ is not a self-adjoint operator on the Hilbert space $\mathcal{H}$, since it can only operate on a restricted subspace of $\mathcal{H}$ as a domain. However, given any operator τ satisfying $[H,\tau] = i\hbar$, we know that $\frac{1}{2}(\tau+\tau^*)$ is a Hermitian operator satisfying this relation.

The Time Delay Operator: Its Domain

By considering the momentum wavefunction at any specified time t_0 we can apply the free particle time operator $t_0 + \frac{1}{2}\frac{m}{\hbar k^2} - \frac{im}{\hbar k}\frac{\partial}{\partial k} + \frac{x_0 m}{\hbar k}$ to make time measurements at the position x_0. As we have seen, the time operator is Hermitian but not self-adjoint. If we construct the time operator for a potential and subtract from it the free particle time operator, we obtain what is known as a time delay operator. If the potential is zero, for example, the time delay operator is the self-adjoint zero operator. It thus may happen that for some potentials, the time delay operator is self-adjoint, or at least Hermitian, with a larger domain than the free particle time operator, for instance. On the other hand, the intersection of time domains for the free particle and the given Hamiltonian may result in a smaller domain for time delay.

Commutator of the Time Delay Operator with the Hamiltonian

Suppose $H = H_0 + H_1$ where $H_0 = \frac{p^2}{2m}$ is the free particle Hamiltonian and $H_1 = V(x)$ is the potential function. Let τ be the time operator corresponding to H and τ_f the free particle time operator. Define $\tau_d = \tau - \tau_f$ as the operator for time delay. Then $[H,\tau] = i\hbar = [H_0,\tau_f]$. Thus we have

$$i\hbar = [H,\tau] = [H_0+H_1,\tau_f+\tau_d] = [H_0,\tau_f] + [H_1,\tau_f] + [H,\tau_d]$$

$$= i\hbar + [H_1,\tau_f] + [H,\tau_d] \ .$$

This shows that $[H,\tau_d] = -[H_1,\tau_f]$.

Since $H_1 = V(x)$ is a function of x it would be useful to express the free particle time operator as an operator on the position wavefunction.

Operator Correspondence and Integration

Our Hilbert space of functions of one real variable corresponding to either one dimensional position or momentum space, consists of functions (complex valued) defined on the range $-\infty < x < +\infty$ with the property that when multiplied by arbitrary polynomials in x or differentiated any number of times the result is square integrable. This insures that the operators x , $-i\frac{\partial}{\partial x}$ on position space and k , $i\frac{\partial}{\partial k}$ on momentum space are self-adjoint. Furthermore, with Fourier transform relating position and momentum wavefunctions we have operator equivalences $x \sim i\frac{\partial}{\partial k}$ and $k \sim -i\frac{\partial}{\partial x}$.

On momentum space, the operator $i\frac{\partial}{\partial k}$ is one to one on functions of k since $i\frac{\partial\phi_1}{\partial k} = i\frac{\partial\phi_2}{\partial k}$ implies ϕ_1 and ϕ_2 differ by a constant which must be zero, since square integrable functions are zero at $\pm\infty$. Thus we can define an inverse of $i\frac{\partial.}{\partial k}$ denoted by $-i\,D_k^{-1}$. It operates as $-i\,D_k^{-1}\phi(k) = -i\int_{-\infty}^{k}\phi(\bar{k})\,d\bar{k}$. Its domain consists of those $\phi(k)$

which satisfy $\int_{-\infty}^{\infty} \phi(k)\, dk = 0$ at least. In fact we insist that every element in the domain of $-i\, D_k^{-1}$ be a derivative of an element already in the Hilbert space.

With this definition, we have the operator equivalences $\frac{1}{k} \sim i\, D_x^{-1}$ and $\frac{1}{k^2} \sim -D_x^{-2}$. With the time operator for the free particle in the form $\tau = t - (\frac{m}{\hbar k})x + \frac{x_0 m}{\hbar k} + \frac{im}{2\hbar k^2}$, as an operator on the position wave function it is

$$\tau = t - i\,\frac{m}{\hbar}\, D_x^{-1} x + i\,\frac{x_0 m}{\hbar}\, D_x^{-1} - i\,\frac{m}{2\hbar}\, D_x^{-2} \,.$$

Thus

$$\tau(\psi(x)) = t\psi(x) - \frac{im}{\hbar}\int_{-\infty}^{x} \bar{x}\psi(\bar{x})dx + \frac{ix_0 m}{\hbar}\int_{-\infty}^{x} \psi(\bar{x})d\bar{x} - \frac{im}{2\hbar}\int_{-\infty}^{x} \left(\int_{-\infty}^{\bar{x}} \psi(\bar{\bar{x}})d\bar{\bar{x}}\right) d\bar{x} \,.$$

The domain of τ consists of those functions ψ for which the above expression exists and defines a function in the Hilbert space. Observe that $D_x^{-1}(x\psi) = \int_{-\infty}^{x} \bar{x}\psi(\bar{x})d\bar{x} = x\, D_x^{-1}\psi - D_x^{-2}\psi$. Thus we also have

$$\begin{aligned}\tau &= t - \frac{imx}{\hbar}\, D_x^{-1} + \frac{ix_0 m}{\hbar}\, D_x^{-1} + \frac{im}{2\hbar}\, D_x^{-2} \\ &= t - \frac{im}{2\hbar}\,(xD_x^{-1} + D_x^{-1}\, x) + \frac{ix_0 m}{\hbar}\, D_x^{-1} \,.\end{aligned}$$

This operates on the position wavefunction $\psi(x,t)$ and corresponds to time measurements at the position x_0. It is Hermitian but not self-adjoint.

Time Delay for Interaction with a Potential:
Example: (The Delta Function Potential in One Dimension.)

The potential $V(x) = V_0\,\delta(x)$ in one dimension has no classical analog. Classically this potential cannot be penetrated, and so measurement of time delay on transmission is meaningless. Let us ask the question what is the time delay for penetration of this potential barrier in quantum mechanics? Let us choose our time domain in such a way that only positive momentum contributions appear for $x > 0$. Observe that approximation methods (like W.K.B. approximation) do not apply to this potential.

The first thing to do is to obtain the energy eigenfunctions $\psi_\omega(x)$ satisfying

$$H\psi_\omega(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_\omega(x) + V_0\delta(x)\psi_\omega(x) = \hbar\omega\psi_\omega(x) \ .$$

By assumption there are only positive momentum contributions for $x > 0$ and so

$$\psi_\omega(x) = A(\omega)\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,x} + B(\omega)\, e^{-i\sqrt{\frac{2m\omega}{\hbar}}\,x} \qquad \text{for} \quad x < 0 \ ,$$

$$= C(\omega)\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,x} \qquad \text{for} \quad x > 0 \ .$$

Continuity at $x = 0 \rightarrow A(\omega) + B(\omega) = C(\omega)$. Discontinuity of $\psi'_\omega(x)$ at $x = 0$, namely $\psi'_\omega(0^+) - \psi'_\omega(0^-) = \frac{2m}{\hbar^2} V_0\psi_\omega(0)$ means

$$\frac{2m}{\hbar^2} V_0\, C(\omega) = i\sqrt{\frac{2m\omega}{\hbar}}\,[C(\omega)-A(\omega)+B(\omega)] = 2i\sqrt{\frac{2m\omega}{\hbar}}\,B(\omega) \ .$$

This gives us the relation $\frac{2m}{\hbar^2} V_0 \, C(\omega) = 2i\sqrt{\frac{2m\omega}{\hbar}} \, B(\omega)$ and so $B(\omega)$ and $C(\omega)$ can be expressed in terms of $A(\omega)$ as

$$B(\omega) = \frac{A(\omega)}{\frac{i\hbar^2}{V_0}\sqrt{\frac{2\omega}{m\hbar}} - 1} \quad , \quad C(\omega) = \frac{A(\omega)}{1 + \frac{iV_0}{\hbar^2}\sqrt{\frac{m\hbar}{2\omega}}} \quad .$$

It only remains to determine $A(\omega)$ in magnitude and phase. The absolute value of $A(\omega)$ is determined from the relation

$$\int_{-\infty}^{\infty} \psi_\omega^*(x) \, \psi_{\omega'}(x)dx = \delta(\omega-\omega') \; .$$

Note that $|A(\omega)|^2 = |B(\omega)|^2 + |C(\omega)|^2$. Let $k = \sqrt{\frac{2m\omega}{\hbar}}$ so $\omega = \frac{\hbar k^2}{2m}$ and $k > 0$; let $k' = \sqrt{\frac{2m\omega'}{\hbar}}$ so $\omega' = \frac{\hbar k'^2}{2m}$, $k' > 0$. We have

$\delta(\omega-\omega') = \delta(\frac{\hbar}{2m}(k^2-k'^2)) = \frac{2m}{\hbar}\delta[(k-k')(k+k')] = \frac{2m}{\hbar 2k}\delta(k-k') = \frac{m}{\hbar k}\delta(k-k')$

for $k,k' > 0$. Now

$$\begin{aligned} \psi_\omega^*(x) &= A^*(\omega)e^{-ikx} + B^*(\omega)e^{ikx} && \text{for } x < 0 \; , \\ &= C^*(\omega)e^{-ikx} && \text{for } x > 0 \; . \\ \psi_{\omega'}(x) &= A(\omega')e^{ik'x} + B(\omega')e^{-ik'x} && \text{for } x < 0 \; , \\ &= C(\omega')e^{ik'x} && \text{for } x > 0 \; . \end{aligned}$$

Now $\int_{-\infty}^{\infty} \psi_\omega^*(x) \, \psi_{\omega'}(x)dx = \frac{m}{\hbar k}\delta(k-k')$. Integrate with respect to k' from

$k-\epsilon$ to $k+\epsilon$ to get $\int_{k-\epsilon}^{k+\epsilon}\int_{-\infty}^{\infty} \psi_{\omega}^{*}(x)\, \psi_{\omega'}(x)dx\, dk' = \frac{m}{\hbar k}$. Consequently, $\frac{m}{\hbar k} = \int_{0}^{\infty}\int_{k-\epsilon}^{k+\epsilon} \psi_{\omega}^{*}(x)\, \psi_{\omega'}(x)dk'\, dx + \int_{-\infty}^{0}\int_{k-\epsilon}^{k+\epsilon} \psi_{\omega}^{*}(x)\, \psi_{\omega'}(x)dk'\, dx$. Applying this result we have $|A(\omega)|^2 = \frac{1}{2\pi}\sqrt{\frac{m}{2\hbar\omega}}$ after integrating. This normalization is general for a local potential in one dimension. The phase of $A(\omega)$ is determined in order to make the eigenfunctions positive and real at the point of arrival. We denote the complete phased, normalized eigenfunction by $\psi_{\omega,x_0}(x)$. It is given by

$$\psi_{\omega,x_0}(x) = \frac{1}{\sqrt{2\pi}}\sqrt[4]{\frac{m}{2\hbar\omega}}\, e^{i\gamma(x_0)}\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,x} + \frac{\frac{1}{\sqrt{2\pi}}\sqrt[4]{\frac{m}{2\hbar\omega}}\, e^{i\gamma(x_0)}}{\frac{i\hbar^2}{V_0}\sqrt{\frac{2\omega}{m\hbar}} - 1}\, e^{-i\sqrt{\frac{2m\omega}{\hbar}}\,x} .$$

for $x < 0$, and

$$\psi_{\omega,x_0}(x) = \frac{\frac{1}{\sqrt{2\pi}}\sqrt[4]{\frac{m}{2\hbar\omega}}\, e^{i\gamma(x_0)}}{1 + \frac{iV_0}{\hbar^2}\sqrt{\frac{m\hbar}{2\omega}}}\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,x} \qquad \text{for} \quad x > 0 .$$

$\gamma(x_0)$ is a real function selected to make the phasing correct. We require $\psi_{\omega,x_0}(x_0) > 0$. This can be divided into two cases, $x_0 > 0$ and $x_0 < 0$. The case $x_0 > 0$ is the simplest one, and is of greatest interest, since we are measuring time delay on transmission through the delta function barrier. For $x_0 > 0$ we have

$$e^{i\gamma(x_0)} = e^{-i\sqrt{\frac{2m\omega}{\hbar}}\,x_0}\,\frac{\left(1 + \frac{iV_0}{\hbar^2}\sqrt{\frac{m\hbar}{2\omega}}\right)}{\sqrt{1 + \frac{mV_0^2}{2\omega\hbar^3}}} ,$$

and from this we can directly get $\psi_{\omega,x_0}(x)$ for the case $x_0 > 0$. It is given by

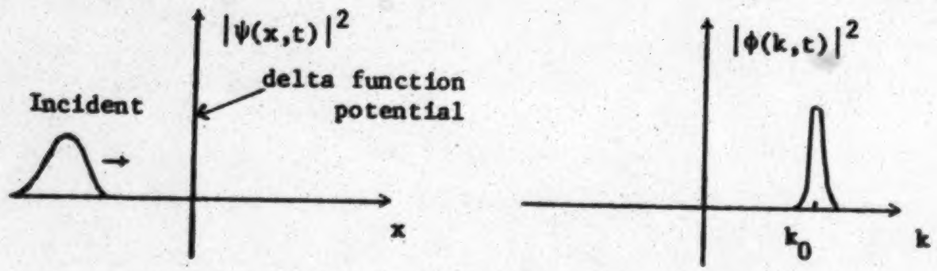
$$\psi_{\omega,x_0}(x) = \frac{1}{\sqrt{2\pi}}\sqrt[4]{\frac{m}{2\hbar\omega}}\,\frac{\left(1 + \frac{iV_0}{\hbar^2}\sqrt{\frac{m\hbar}{2\omega}}\right)}{\sqrt{1 + \frac{mV_0^2}{2\omega\hbar^3}}}\,e^{i\sqrt{\frac{2m\omega}{\hbar}}\,(x-x_0)}$$

$$+ \frac{\frac{1}{\sqrt{2\pi}}\sqrt[4]{\frac{m}{2\hbar\omega}}\left(1 + \frac{iV_0}{\hbar^2}\sqrt{\frac{m\hbar}{2\omega}}\right)}{\left(\frac{i\hbar^2}{V_0}\sqrt{\frac{2\omega}{m\hbar}} - 1\right)\sqrt{1 + \frac{mV_0^2}{2\omega\hbar^3}}}\,e^{-i\sqrt{\frac{2m\omega}{\hbar}}\,(x+x_0)}$$

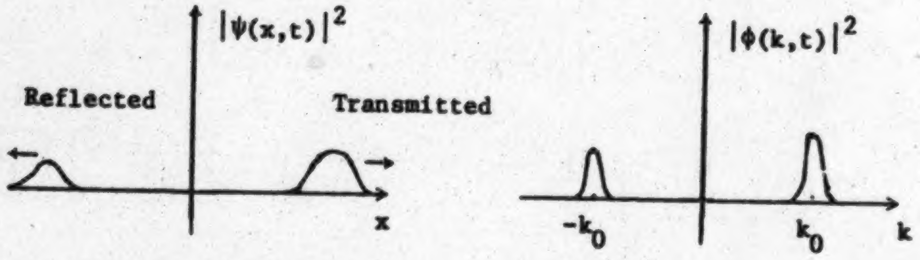
for $x < 0$ and by

$$\psi_{\omega,x_0}(x) = \frac{\frac{1}{\sqrt{2\pi}}\sqrt[4]{\frac{m}{2\hbar\omega}}}{\sqrt{1 + \frac{mV_0^2}{2\omega\hbar^3}}}\,e^{i\sqrt{\frac{2m\omega}{\hbar}}\,(x-x_0)} \quad \text{for} \quad x > 0 .$$

In this time domain we are considering wave packets with a positive momentum distribution that are being scattered from a delta function potential. We can sketch the (absolute value squared of the) position and momentum wavefunctions before and after scattering.


$|\psi(x,t)|^2$
Incident
delta function potential
x
$|\phi(k,t)|^2$
k_0
k

Before scattering - position and momentum wavefunctions


$|\psi(x,t)|^2$
Reflected
Transmitted
x
$|\phi(k,t)|^2$
$-k_0$
k_0
k

After scattering - position and momentum wavefunctions

Figure 17

Delta Function Scattering

Let us take a point $x_0 > 0$ and look at the expected time of arrival of the transmitted wave packet for the delta function potential, and the expected time of arrival for the same incident wave packet at x_0 if the potential $V(x)$ had not existed. The difference between this two values for narrow momentum distribution about $k_0 > 0$ gives us the time delay in terms of k_0. Let the wave packet be completely determined from the general position wavefunction

$$\psi(x,t) = \int_0^\infty A(\omega,x_0)\, \psi_{\omega,x_0}(x)\, e^{-i\omega t}\, d\omega \;.$$

We assume $|A(\omega,x_0)|^2$ (which is independent of x_0) is a narrow distribution about $\omega_0 = \frac{\hbar k_0^2}{2m}$. The expected time of arrival at $x_0 > 0$ is $\langle t\rangle_{x_0} = \int_0^\infty A^*(\omega,x_0)[-i\frac{\partial}{\partial\omega}] A(\omega,x_0)d\omega$. Here we assume that $\psi(x,t)$ is normalized, i.e. $\int_{-\infty}^\infty |\psi(x,t)|^2 \, d\,x = 1$ so that $A(\omega,x_0)$ is normalized, i.e. $\int_0^\infty |A(\omega,x_0)|^2 \, d\omega = 1$.

Recall that we wrote the energy eigenfunctions in the form

$$\begin{aligned}\psi_\omega(x) &= A(\omega)\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,x} + B(\omega)\, e^{-i\sqrt{\frac{2m\omega}{\hbar}}\,x} \qquad \text{for} \quad x < 0 \ , \\ &= C(\omega)\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,x} \qquad \text{for} \quad x > 0 \ .\end{aligned}$$

When we take superposition, the $A(\omega)$ terms form the incident wave packet, $B(\omega)$ the reflected wave packet and $C(\omega)$ the transmitted wave packet. In the equation

$$\psi(x,t) = \int_0^\infty A(\omega,x_0)\ \psi_{\omega,x_0}(x)\ e^{-i\omega t}\ d\omega$$

for sufficiently large past time (negative t) only the incident wave packet of the eigenfunctions $\psi_{\omega,x_0}(x)$ contributes. Hence if we let $\psi_1(x,t)$ denote the free particle wave function asymptotic to $\psi(x,t)$ for $t \to -\infty$, we have

$$\psi_1(x,t) = \int_0^\infty A(\omega,x_0)\left[\frac{1}{\sqrt{2\pi}}\sqrt[4]{\frac{m}{2\hbar\omega}}\;\frac{\left(1 + \frac{iV_0}{\hbar^2}\sqrt{\frac{m\hbar}{2\omega}}\right)}{\sqrt{1 + \frac{mV_0^2}{2\omega\hbar^3}}}\;e^{i\sqrt{\frac{2m\omega}{\hbar}}(x-x_0)}\right]e^{-i\omega t}\,d\omega\,.$$

Now let us ask what is the expected time of arrival for this wave packet for a free particle at the point x_0. Let $\psi^f_{\omega,x_0}(x)$ denote the energy eigenfunctions for a free particle in one dimension with positive momentum distribution phased at x_0. Let $A^f(\omega,x_0)$ denote the energy distribution for $\psi_1(x,t)$. Then

$$\psi_1(x,t) = \int_0^\infty A^f(\omega,x_0)\,\psi^f_{\omega,x_0}(x)\,e^{-i\omega t}\,d\omega\,.$$

Recall that

$$\psi^f_{\omega,x_0}(x) = \frac{1}{\sqrt{2\pi}}\sqrt[4]{\frac{m}{2\hbar\omega}}\;e^{i\sqrt{\frac{2m\omega}{\hbar}}(x-x_0)}$$

which we derived earlier. Consequently

$$A^f(\omega,x_0) = A(\omega,x_0)\;\frac{\left(1 + \frac{iV_0}{\hbar^2}\sqrt{\frac{m\hbar}{2\omega}}\right)}{\sqrt{1 + \frac{mV_0^2}{2\omega\hbar^3}}}\,.$$

The expected arrival time for the free particle described by $\psi_1(x,t)$ at the point x_0 is given by

$$\langle t\rangle^f_{x_0} = \int_0^\infty A^{f^*}(\omega,x_0)\left[-i\frac{\partial}{\partial\omega}\right]A^f(\omega,x_0)\,d\omega\,.$$

The time delay Δt for the interaction with the delta function potential is

$$\Delta t = \langle t\rangle_{x_0} - \langle t\rangle^{f}_{x_0}$$

$$= \int_0^\infty A^*(\omega,x_0)\left[-i \frac{\partial}{\partial\omega}\right] A(\omega,x_0)\,d\omega - \int_0^\infty A^{f^*}(\omega,x_0)\left[-i \frac{\partial}{\partial\omega}\right] A^f(\omega,x_0)\,d\omega$$

$$= \frac{\dfrac{V_0 m}{4\hbar\omega_0^2}\left(\dfrac{2\omega_0}{m\hbar}\right)^{1/2}}{1 + \dfrac{mV_0^2}{2\omega_0\hbar^3}}$$

for a narrow energy distribution $|A(\omega,x_0)|^2$, about ω_0. Expressing Δt in terms of $k_0 = \sqrt{\dfrac{2m\omega_0}{\hbar}}$ we get $\Delta t = \dfrac{V_0 m^2 \hbar}{k_0(\hbar^4 k_0^2 + m^2 V_0^2)}$,

as the time delay for the interaction of a very narrow wave packet in momentum space distributed about $k_0 > 0$ with the delta function potential $V(x) = V_0\,\delta(x)$. If the range of the potential $V(x)$ is much smaller than the wavelength $\dfrac{2\pi}{k_0}$, this expression will be a good approximation in general.

General Relation Between Time Delay and the Phase of the Transmission Coefficient for the Momentum Transformation Kernel

Consider a local potential $V(x)$ in one dimension defined on the range $-a < x < a$. We have solutions $\psi(x)$ to the Schrödinger equation with the behavior

$$\psi(x) = \frac{1}{\sqrt{2\pi}} e^{ik_0 x} + B(k_0)\, e^{-ik_0 x} \qquad \text{for} \quad x < -a$$

$$= C(k_0)\, e^{ik_0 x} \qquad \text{for} \quad x > a \quad ,$$

for each $k_0 > 0$. For $x > a$ we have only positive momentum contributions indicating that the initial wave packet before scattering had only positive momenta in its makeup.

The functions $B(k)$ and $C(k)$ are determined if the potential is specified. They satisfy $2\pi(|B(k)|^2 + |C(k)|^2) = 1$ for all k. The momentum transformation kernel is $B_t(k,k_0) = \sqrt{2\pi}\,(B(k_0)\delta(k+k_0) + C(k_0)\delta(k-k_0))$.

Let us determine the energy eigenfunctions $\psi_{\omega,x_0}(x)$ in this particular time domain. Without normalization we have

$$\psi_\omega(x) = \frac{1}{\sqrt{2\pi}} e^{i\sqrt{\frac{2m\omega}{\hbar}}\,x} + B\left(\sqrt{\frac{2m\omega}{\hbar}}\right) e^{-i\sqrt{\frac{2m\omega}{\hbar}}\,x} \qquad \text{for} \quad x < -a$$

$$= C\left(\sqrt{\frac{2m\omega}{\hbar}}\right) e^{i\sqrt{\frac{2m\omega}{\hbar}}\,x} \qquad \text{for} \quad x > a \quad .$$

We normalize so that $\int_{-\infty}^{\infty} \psi_\omega^*(x)\, \psi_{\omega'}(x)dx = \delta(\omega-\omega')$. An important result to note is that this normalization is independent of the local details of the potential. The incident $(A(\omega))$ term always satisfies

$|A(\omega)|^2 = \frac{1}{2\pi}\sqrt{\frac{m}{2\hbar\omega}}$. Consequently, the normalized energy eigenfunction in our time domain is

$$\psi_\omega(x) = \frac{1}{\sqrt{2\pi}}\sqrt[4]{\frac{m}{2\hbar\omega}}\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,x} + B\left(\sqrt{\frac{2m\omega}{\hbar}}\right)\sqrt[4]{\frac{m}{2\hbar\omega}}\, e^{-i\sqrt{\frac{2m\omega}{\hbar}}\,x} \qquad \text{for} \quad x \leq -a ,$$

$$= C\left(\sqrt{\frac{2m\omega}{\hbar}}\right)\sqrt[4]{\frac{m}{2\hbar\omega}}\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,x} \qquad \text{for} \quad x > a .$$

The behavior of $\psi_\omega(x)$ on the interval $-a \leq x < a$ is of no concern to us here. The only thing left to do is to phase the energy eigenfunctions at a point $x_0 > 0$ (or in this case, a point $x_0 > a$) . Doing this we obtain

$$\psi_{\omega,x_0}(x) = \frac{1}{\sqrt{2\pi}}\sqrt[4]{\frac{m}{2\hbar\omega}}\,\frac{C^*\left(\sqrt{\frac{2m\omega}{\hbar}}\right)}{\left|C\left(\sqrt{\frac{2m\omega}{\hbar}}\right)\right|}\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,(x-x_0)}$$

$$+ B\left(\sqrt{\frac{2m\omega}{\hbar}}\right)\sqrt[4]{\frac{m}{2\hbar\omega}}\,\frac{C^*\left(\sqrt{\frac{2m\omega}{\hbar}}\right)}{\left|C\left(\sqrt{\frac{2m\omega}{\hbar}}\right)\right|}\, e^{-i\sqrt{\frac{2m\omega}{\hbar}}\,(x+x_0)} \qquad \text{for} \quad x < a ,$$

$$\psi_{\omega,x_0}(x) = \left|C\left(\sqrt{\frac{2m\omega}{\hbar}}\right)\right|\sqrt[4]{\frac{m}{2\hbar\omega}}\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,(x-x_0)} \qquad \text{for} \quad x > a .$$

Now consider a general wavefunction $\psi(x,t)$ expanded in energy eigenfunctions as $\psi(x,t) = \int_0^\infty A(\omega,x_0)\,\psi_{\omega,x_0}(x)\,e^{-i\omega t}\,d\omega$. We suppose $|A(\omega,x_0)|^2$ is a narrow distribution about ω_0 , and $\psi(x,t)$ describes a scattering interaction. Let $\psi_1(x,t)$ be the free particle wave function whose wave packet coincides with that of $\psi(x,t)$ for sufficiently large negative t . Only the incident waves in the energy eigenfunctions contribute to the actual wave function $\psi(x,t)$ before scattering, and so

$$\psi_1(x,t) = \int_0^\infty A(\omega,x_0) \left[\frac{1}{\sqrt{2\pi}}\sqrt[4]{\frac{m}{2\hbar\omega}}\, \frac{C^*(\sqrt{\frac{2m\omega}{\hbar}})}{|C(\sqrt{\frac{2m\omega}{\hbar}})|}\, e^{i\sqrt{\frac{2m\omega}{\hbar}}(x-x_0)}\right] e^{-i\omega t}\, d\omega \, .$$

As in the case of the delta function potential, $\psi_1(x,t)$ can be expanded in free particle energy eigenfunctions

$$\psi_1(x,t) = \int_C^\infty A^f(\omega,x_0)\, \psi^f_{\omega,x_0}(x)\, e^{-i\omega t}\, d\omega \quad .$$

Using

$$\psi^f_{\omega,x_0}(x) = \frac{1}{\sqrt{2\pi}}\sqrt[4]{\frac{m}{2\hbar\omega}}\, e^{i\sqrt{\frac{2m\omega}{\hbar}}(x-x_0)}$$

we get

$$A^f(\omega,x_0) = A(\omega,x_0)\, \frac{C^*(\sqrt{\frac{2m\omega}{\hbar}})}{|C(\sqrt{\frac{2m\omega}{\hbar}})|} \quad .$$

From this we can derive a relation between the phase of the function C(k) and the time delay as follows.

$$\Delta t = \langle t\rangle_{x_0} - \langle t\rangle^f_{x_0}$$

$$= \int_0^\infty A^*(\omega,x_0)[-i\tfrac{\partial}{\partial\omega}]A(\omega,x_0)d\omega - \int_0^\infty A^{f*}(\omega,x_0)[-i\tfrac{\partial}{\partial\omega}]\, A^f(\omega,x_0)d\omega$$

$$= \int_0^\infty A^*(\frac{\hbar k^2}{2m}, x_0)[-i \frac{\partial}{\partial k}]A(\frac{\hbar k^2}{2m}, x_0)dk - \int_0^\infty A^{f^*}(\frac{\hbar k^2}{2m}, x_0)[-i \frac{\partial}{\partial k}]A^f(\frac{\hbar k^2}{2m}, x_0)dk$$

$$= \int_0^\infty |A(\frac{\hbar k^2}{2m}, x_0)|^2 \frac{C(k)}{|C(k)|} (i \frac{\partial}{\partial k})\{\frac{C^*(k)}{|C(k)|}\} dk$$

$$= \int_0^\infty \frac{m}{\hbar k_0} \delta(k-k_0) \frac{C(k)}{|C(k)|} (i \frac{\partial}{\partial k}) \{\frac{C^*(k)}{|C(k)|}\} dk$$ for narrow distributions of energies about $\omega_0 = \hbar k_0^2/2m$

$$= \frac{m}{\hbar k_0} \frac{C(k_0)}{|C(k_0)|} (i \frac{\partial}{\partial k_0}) \{\frac{C^*(k_0)}{|C(k_0)|}\} .$$

Let us suppose that $\frac{C(k_0)}{|C(k_0)|} = e^{+i\lambda(k_0)}$. We can easily check that $\Delta t = \frac{m\lambda'(k_0)}{\hbar k_0}$ where $\lambda'(k_0) = \frac{d\lambda}{dk_0}$. This means that knowing time delay Δt as a function of initial momentum, we can determine the phase of the transmission coefficient C from $\lambda(k_0) = \frac{\hbar}{m}\int k_0 \, \Delta t(k_0) \, dk_0$.

Transmission Only

The time delay Δt can be determined by an alternate method in the special case of transmission only (no reflection) in one dimensional scattering. In this case the momentum transformation kernel is $B_t(k,k_0) = \sqrt{2\pi}\, C(k_0)\, \delta(k-k_0)$ and so $\phi_2(k,t) = \sqrt{2\pi}\, C(k)\, \phi_1(k,t)$ where $2\pi|C(k)|^2 = 1$ for all k . Let $e^{i\lambda(k)} = \frac{C(k)}{|C(k)|} = \sqrt{2\pi}\, C(k)$. Then $C(k) = \frac{1}{\sqrt{2\pi}} e^{i\lambda(k)}$ and so $\phi_2(k,t) = e^{i\lambda(k)} \phi_1(k,t)$. Observe that ϕ_1 and hence ϕ_2 are zero for negative k . Using the free particle time of arrival operator, namely $t - \frac{im}{\hbar k}\frac{\partial}{\partial k} + \frac{x_o m}{\hbar k} + \frac{im}{2\hbar k^2}$ we can determine the time delay as

$$\Delta t = \langle t\rangle^2_{x_0} - \langle t\rangle^1_{x_0}$$

$$= \int_0^\infty \phi_2^*(k,t)\,[t - \frac{im}{\hbar k}\frac{\partial}{\partial k} + \frac{x_0 m}{\hbar k} + \frac{im}{2\hbar k^2}]\,\phi_2(k,t)\,dk$$

$$- \int_0^\infty \phi_1^*(k,t)\,[t - \frac{im}{\hbar k}\frac{\partial}{\partial k} + \frac{x_0 m}{\hbar k} + \frac{im}{2\hbar k^2}]\,\phi_1(k,t)\,dk$$

$$= -\frac{im}{\hbar}\int_0^\infty \frac{\phi_2^*(k,t)}{k}\frac{\partial}{\partial k}\phi_2(k,t)dk + \frac{im}{\hbar}\int_0^\infty \frac{\phi_1^*(k,t)}{k}\frac{\partial}{\partial k}\phi_1(k,t)\,dk$$

$$= -\frac{im}{\hbar}\int_0^\infty \frac{e^{-i\lambda(k)}\;\phi_1^*(k,t)}{k}\frac{\partial}{\partial k}\{e^{i\lambda(k)}\;\phi_1(k,t)\}\,dk + \frac{im}{\hbar}\int_0^\infty \frac{\phi_1^*(k,t)}{k}\frac{\partial}{\partial k}\phi_1(k,t)dk$$

$$= -\frac{im}{\hbar}\int_0^\infty \frac{e^{-i\lambda(k)}}{k}\,|\phi_1(k,t)|^2\;i\lambda'(k)\;e^{i\lambda(k)}\,dk$$

$$= \frac{m}{\hbar k_0}\lambda'(k_0)$$, for narrow distributions about k_0 .

This expression $\Delta t = \frac{m}{\hbar k_0}\lambda'(k_0)$ derived in the special case of transmission only, is the same as the more general result which we obtained earlier.

CHAPTER VIII

NORMALIZATION IN THREE DIMENSIONS

Let us consider the eigenfunction normalization equation in three dimensions, namely $\int_{\text{space}} \psi^*_{\omega}(\vec{r})\psi_{\omega'}(\vec{r})\, d\vec{r} = \delta(\omega-\omega')$.

As an example, consider the free particle in 3 dimensions. The momentum eigenfunctions $\psi_{\vec{k}}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}}$ are normalized in the sense that $\int_{\text{space}} \psi^*_{\vec{k}}(\vec{r})\, \psi_{\vec{k}'}(\vec{r})\, d\vec{r} = \delta(\vec{k}-\vec{k}')$. Now suppose we examine a time domain and impose ω normalization. If we take the simplest case imaginable (and one that is useful in scattering theory) namely the time domain of all negative momenta $\vec{k}$ directed along the z axis, $\vec{k} = -k\hat{z}$, $k > 0$, we must normalize

$$\psi_{\omega}(\vec{r}) = \frac{1}{(2\pi)^{3/2}}\, e^{-i\sqrt{\frac{2m\omega}{\hbar}}\, z}$$

with an integration over all space. This is clearly impossible since $\psi_{\omega}(\vec{r})$ is independent of x and y and these integrations will diverge. It is therefore necessary to consider solid angle distributions in momentum space. We write

$$\psi_{\omega}(\vec{r}) = \int_{\hat{k}} A_{\omega}(\hat{k})\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,\hat{k}\cdot\vec{r}}\, d\Omega_{\hat{k}} \quad ,$$

for the free particle in three dimensions. $\hat{k}$ is a unit vector specifying the direction of momentum. We now substitute this expression for $\psi_\omega(\vec{r})$ into the normalization integral $\int_{\text{space}} \psi^*_\omega(\vec{r})\psi_{\omega'}(\vec{r})\, d\vec{r} = \delta(\omega-\omega')$ to get

$$\int_{\text{space}} \psi^*_\omega(\vec{r})\psi_{\omega'}(\vec{r})d\vec{r} = (2\pi)^3 \int_{\hat{k}}\int_{\hat{k}'} A^*_\omega(\hat{k})A_{\omega'}(\hat{k}')\delta\left(\sqrt{\frac{2m\omega'}{\hbar}}\,\hat{k}' - \sqrt{\frac{2m\omega}{\hbar}}\,\hat{k}\right) d\Omega_{\hat{k}}\, d\Omega_{\hat{k}'} ,$$

so

$$\frac{m}{\hbar k}\,\delta(k-k') = (2\pi)^3 \int_{\hat{k}}\int_{\hat{k}'} A^*_\omega(\hat{k})A_{\omega'}(\hat{k}')\delta(k'\hat{k}'-k\hat{k})\, d\Omega_{\hat{k}}\, d\Omega_{\hat{k}'} .$$

The volume element in momentum space is $k'^2\, dk'\, d\Omega_{\hat{k}'}$. Multiply by $k'^2\, dk'$ and integrate to get

$$\frac{mk}{\hbar} = (2\pi)^3 \int_k |A_\omega(\hat{k})|^2\, d\Omega_{\hat{k}} .$$

or alternatively

$$\int_{\hat{k}} |A_\omega(k)|^2\, d\Omega_k = \frac{m}{(2\pi)^3\hbar}\sqrt{\frac{2m\omega}{\hbar}} .$$

This is the normalization condition which must be imposed on the solid angle expansion coefficients $A_\omega(\hat{k})$ in the energy eigenfunction $\psi_\omega(\vec{r})$ for the free particle in three dimensions

$$\psi_\omega(\vec{r}) = \int_{\hat{k}} A_\omega(\hat{k})\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,\hat{k}\cdot\vec{r}}\, d\Omega_{\hat{k}}$$

in order that the normalization $\int_{\text{space}} \psi^*_\omega(\vec{r})\psi_{\omega'}(\vec{r})\, d\vec{r} = \delta(\omega-\omega')$ will hold. The condition is necessary and sufficient.

Specifying $A_\omega(\hat{k})$ satisfying the normalization coeffient for all $\omega > 0$ determines a time domain for the free particle in three dimensions.

The direction of $\hat{k}$ can be specified by two spherical angles θ_k and ϕ_k so that $A_\omega(\hat{k}) = A_\omega(\theta_k,\phi_k)$, and

$$\int_{\hat{k}} |A_\omega(k)|^2 \, d\Omega_{\hat{k}} = \int_{\theta_k=0}^{\pi} \int_{\phi_k=0}^{2\pi} |A_\omega(\theta_k,\phi_k)|^2 \sin\theta_k \, d\theta_k \, d\phi_k$$

$$= \frac{m}{(2\pi)^3 \hbar} \sqrt{\frac{2m\omega}{\hbar}} \ .$$

In the case where $A_\omega(\theta_k,\phi_k)$ is independent of ϕ_k we have

$$\int_{\theta_k=0}^{\pi} |A_\omega(\theta_k)|^2 \sin\theta_k \, d\theta_k = \frac{m}{(2\pi)^4 \hbar} \sqrt{\frac{2m\omega}{\hbar}} \ .$$

In general, we suppose $A_\omega(\theta_k)$ is zero except for a very narrow range of values of θ_k near $\theta_k = \pi$. For such narrow distributions,

$$|A_\omega(\theta_k)|^2 = \frac{2\delta(1 + \cos\theta_k)m}{(2\pi)^4 \hbar} \sqrt{\frac{2m\omega}{\hbar}} \ .$$

Let us take a particular form for the delta function in this case $\delta(x) = \frac{1}{2\epsilon}$ for $|x| < \epsilon$ and $\delta(x) = 0$ for $|x| > \epsilon$ where $\epsilon > 0$ is small. Thus we see that

$$|A_\omega(\theta_k)|^2 = \frac{m}{(2\pi)^4 \hbar\epsilon} \sqrt{\frac{2m\omega}{\hbar}} \quad \text{for } \overline{\theta}_L < \theta_k \leq \pi$$

where $\bar{\theta}_L$ satisfies $1 + \cos\bar{\theta}_L = \epsilon$, and $|A_\omega(\theta_k)|^2 = 0$ for $0 < \theta_k < \bar{\theta}_L$.

Now let us consider the actual value $A_\omega(\theta_k)$. When we take the square root above there is a phase uncertainty of the form $e^{i\gamma(\omega,\theta_k)}$. The ω dependence is unimportant, since this directly relates to the phasing of $\psi_\omega(\vec{r})$ which is to be determined later by phasing at point of arrival. The θ_k dependence is insignificant, since the distribution is narrow in θ_k near π . We ignore the phasing, and set

$$A_\omega(\theta_k) = \frac{1}{(2\pi)^2}\sqrt{\frac{m}{\hbar\epsilon}}\sqrt[4]{\frac{2m\omega}{\hbar}} \quad \text{for } \bar{\theta}_L < \theta_k < \pi \ ,$$

$$= 0 \quad \text{for } 0 < \theta_k < \bar{\theta}_L \ .$$

We substitute this back into the expression

$$\psi_\omega(\vec{r}) = \int_{\hat{k}} A_\omega(\hat{k})\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,\hat{k}\cdot\vec{r}}\, d\Omega_{\hat{k}} \ ,$$

to get

$$\psi_\omega(\vec{r}) = \frac{1}{(2\pi)^2}\sqrt{\frac{m}{\hbar\epsilon}}\sqrt[4]{\frac{2m\omega}{\hbar}}\int_{\theta_k=\bar{\theta}_L}^{\pi}\int_{\phi_k=0}^{2\pi}$$

$$e^{i\sqrt{\frac{2m\omega}{\hbar}}(x\sin\theta_k\cos\phi_k + y\sin\theta_k\sin\phi_k + z\cos\theta_k)}\sin\theta_k d\theta_k d\phi_k \ .$$

This is an exact expression. Now we begin approximation. First of all, let us suppose that the terms involving $\cos\phi_k$ and $\sin\phi_k$ give insignificant contributions that can be neglected. This means that

$\sqrt{\frac{2m\omega}{\hbar}} \sin \bar{\theta}_L << \frac{1}{|x|}$ and much less than $\frac{1}{|y|}$. The locality bounds on x and y are $|x|$ and $|y| << \frac{1}{2}\sqrt{\frac{\hbar}{m\omega\epsilon}}$. For x and y satisfying these locality bounds, $\psi_\omega(\vec{r})$ can be written as

$$\psi_\omega(\vec{r}) = \frac{1}{2\pi}\sqrt{\frac{m}{\hbar\epsilon}}\sqrt[4]{\frac{2m\omega}{\hbar}}\int_{\theta_k=\bar{\theta}_L}^{\pi} e^{i\sqrt{\frac{2m\omega}{\hbar}}\, z\cos\theta_k}\sin\theta_k \, d\theta_k$$

$$= \frac{e^{-i\sqrt{\frac{2m\omega}{\hbar}}\, z}}{-i\sqrt{\frac{2m\omega}{\hbar}}\, z}\left(1 - e^{i\sqrt{\frac{2m\omega}{\hbar}}\, z\epsilon}\right)\frac{1}{2\pi}\sqrt{\frac{m}{\hbar\epsilon}}\sqrt[4]{\frac{2m\omega}{\hbar}} \quad .$$

As a final approximation, we assume $|z| << \frac{1}{\epsilon}\sqrt{\frac{\hbar}{2m\omega}}$. In this case

$$\psi_\omega(\vec{r}) = \frac{1}{2\pi}\sqrt{\frac{m\epsilon}{\hbar}}\sqrt[4]{\frac{2m\omega}{\hbar}}\, e^{-i\sqrt{\frac{2m\omega}{\hbar}}\, z} \quad .$$

This is valid for $|x|$, $|y| << \frac{1}{2}\sqrt{\frac{\hbar}{m\omega\epsilon}}$ and $|z| << \frac{1}{\epsilon}\sqrt{\frac{\hbar}{2m\omega}}$. It has the form $e^{-i\sqrt{\frac{2m\omega}{\hbar}}\, z}$ as required, but as $\epsilon \to 0$ the amplitude of $\psi_\omega(\vec{r})$ degenerates uniformly to zero. This explains the problems we encountered in trying to normalize $e^{-i\sqrt{\frac{2m\omega}{\hbar}}\, z}$ in the variable ω using spatial integration. ϵ specifies over what range $\psi_\omega(\vec{r})$ behaves like plane waves, and it gives the amplitude of these waves in that region. We see for larger regions of plane wave behavior we have smaller ϵ and consequently less amplitude.

For $k = \sqrt{\frac{2m\omega}{\hbar}}$ and for momenta directed along the z axis in a positive direction we have

$$\psi_{\omega}(\vec{r}) = \frac{1}{2\pi} \sqrt{\frac{m\epsilon}{\hbar}}\, k^{1/2}\, e^{ikz} \quad ,$$

for x , y , z satisfying the restrictions above.

CHAPTER IX

EIGENFUNCTION PHASING IN TIME OF ARRIVAL

Let $\psi(\vec{r},t)$ be expanded in evergy eigenfunctions as

$$\psi(\vec{r},t) = \int_0^\infty A(\omega,\vec{r}_0)\psi_{\omega,\vec{r}_0}(\vec{r})\, e^{-i\omega t} d\omega = \int_0^\infty A(\omega)\psi_\omega(\vec{r})\, e^{-i\omega t}\, d\omega \; .$$

Let $\psi_{\omega,\vec{r}_0}(\vec{r}) = \psi_\omega(\vec{r})\, e^{i\gamma_\omega(\vec{r}_0)}$ and $A(\omega,\vec{r}_0) = A(\omega)\, e^{-i\gamma_\omega(\vec{r}_0)}$ where $\gamma_\omega(\vec{r}_0)$ is the eigenfunction phase term. If we choose eigenfunction point phasing for instance, $e^{i\gamma_\omega(\vec{r}_0)} = \dfrac{\psi^*_\omega(\vec{r}_0)}{|\psi_\omega(\vec{r}_0)|}$. For linearity between $\psi(\vec{r},t)$ and $A(\omega,\vec{r}_0)$ on the time domain, we require that the phasing of the eigenfunction $\psi_\omega(\vec{r})$ depends only on the eigenfunctions and not on the explicit wavefunction or energy amplitude function.

Now $\langle t\rangle_{\vec{r}_0} = \int_0^\infty A^*(\omega,\vec{r}_0)(-i \frac{\partial}{\partial\omega}) A(\omega,\vec{r}_0)\, d\omega$. Let us take $A(\omega)$ to be the normalized narrow distribution $A(\omega) = \sqrt{\delta(\omega-\omega_0)}$. Then $A(\omega,\vec{r}_0) = \sqrt{\delta(\omega-\omega_0)}\; \exp(-i\gamma_\omega(\vec{r}_0))$ and so

$$\langle t\rangle_{\vec{r}_0} = \int_0^\infty \sqrt{\delta(\omega-\omega_0)}\; e^{+i\gamma_\omega(\vec{r}_0)}(-i\frac{\partial}{\partial\omega})[\sqrt{\delta(\omega-\omega_0)}\; e^{-i\gamma_\omega(\vec{r}_0)}]\, d\omega$$

$$= \int_0^\infty \sqrt{\delta(\omega-\omega_0)}\; (-i)\, \frac{1}{2}\, (\delta(\omega-\omega_0))^{-1/2}\; \delta'(\omega-\omega_0)\, d\omega$$

$$+ \int_0^\infty \delta(\omega-\omega_0)\, e^{i\gamma_\omega(\vec{r}_0)} (-i)\, e^{-i\gamma_\omega(\vec{r}_0)} \left(-i \frac{\partial}{\partial\omega} \gamma_\omega(\vec{r}_0)\right) d\omega$$

$$= - \frac{\partial}{\partial\omega_0} (\gamma_{\omega_0}(\vec{r}_0)) \quad .$$

From this we can examine $\nabla_{\vec{r}_0} (\langle t\rangle_{\vec{r}_0}) = - \frac{\partial}{\partial\omega_0} (\nabla_{\vec{r}_0} \gamma_{\omega_0}(\vec{r}_0))$ the gradient vector of maximum time variation.

Suppose now we are considering scattering from a local potential near $\vec{r} = 0$ in three dimensions, and the detector is a great distance from the scattering centre, and is off at an angle and out of the influence of incident waves that miss or do not interact with the potential. The detector region only contains spherical outgoing waves. Suppose we are measuring time of arrival at the detector. Let the detector be located at $\vec{r}_0$. For elastic scattering, the momentum magnitude of the particle measured at $\vec{r}_0$ will be $k_0 = \sqrt{\frac{2m\omega_0}{\hbar}}$ and the direction of momentum will be $\hat{r}_0 = \frac{\vec{r}_0}{|\vec{r}_0|}$. We insist that the gradient vector of maximum time variation be in the direction $\hat{r}_0$ with magnitude $\frac{1}{v_0} = \frac{m}{\hbar k_0} = \sqrt{\frac{m}{2\omega_0\hbar}}$. Thus

$$- \frac{\partial}{\partial\omega_0} (\nabla_{\vec{r}_0} \gamma_{\omega_0}(\vec{r}_0)) = \sqrt{\frac{m}{2\omega_0\hbar}} \; \frac{\vec{r}_0}{|\vec{r}_0|} \quad .$$

Since the gradient is radially directed, $\gamma_{\omega_0}(\vec{r}_0)$ is a function only of r_0 the magnitude of $\vec{r}_0$ (and of course ω_0). Hence

$$- \frac{\partial}{\partial\omega_0} (\gamma_{\omega_0}(\vec{r}_0)) = \sqrt{\frac{m}{2\omega_0\hbar}} \; (r_0 + f(\omega_0)) = \langle t \rangle_{\vec{r}_0} \; .$$

For the moment, let us provisionally ignore the term $f(\omega_0)$ which is related to the setting of the clock and let $\gamma_{\omega_0}(\vec{r}_0)$ be proportional to r_0 . We have $- \frac{\partial}{\partial\omega_0} (\gamma_{\omega_0}(\vec{r}_0)) = \sqrt{\frac{m}{2\omega_0\hbar}}\, r_0$ and so $\gamma_{\omega_0}(\vec{r}_0) = -\sqrt{\frac{2m\omega_0}{\hbar}}\, r_0 = -k_0 \, r_0$. This means that $\psi_{\omega_0,\vec{r}_0}(\vec{r}) \simeq \psi_{\omega_0}(\vec{r}) \, e^{-ik_0 r_0}$. Suppose $\psi_{\omega_0}(\vec{r}) \simeq \frac{e^{i\sqrt{\frac{2m\omega_0}{\hbar}}\, r}}{r} = \frac{e^{ik_0 r}}{r}$. Then $\psi_{\omega_0,\vec{r}_0}(\vec{r}) \simeq \frac{e^{ik_0(r-r_0)}}{r}$ which is positive at $r = r_0$. This is seen as a justification of eigenfunction point phasing.

CHAPTER X

NOTES ON ORTHOGONALITY OF TIME EIGENFUNCTIONS

Allcock[1] discusses the inherent problems in measuring time of arrival in quantum mechanics. One of his observations is that it is impossible to find a set of functions $\psi_t(\omega)$ which are eigenfunctions of the time operator $-i\frac{\partial}{\partial\omega}$ and which are orthogonal in the sense that $\int_0^\infty \psi_t^*(\omega)\psi_{t'}(\omega)d\omega = \delta(t-t')$. This is true in general, however if we take $\psi_t(\omega) = \frac{1}{\sqrt{2\pi}}\, e^{i\omega t}$ we satisfy the eigenvalue equation $-i\frac{\partial}{\partial\omega}\psi_t(\omega) = t\psi_t(\omega)$. The orthogonality relation becomes $\delta(t-t') = \frac{1}{2\pi}\int_0^\infty e^{i\omega(t'-t)}\, d\omega$. The fact is, this integral does behave like a delta function (identity) transformation when it operates on the domain of time amplitude functions. If $T(t',x_0)$ is a time amplitude function, then

$$\int_{-\infty}^\infty \left[\frac{1}{2\pi}\int_0^\infty e^{i\omega(t'-t)}d\omega\right] T(t',x_0)\, dt'$$

$$= \frac{1}{\sqrt{2\pi}}\int_0^\infty e^{-i\omega t}\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^\infty e^{i\omega t'}\, T(t',x_0)dt'\right)d\omega = \frac{1}{\sqrt{2\pi}}\int_0^\infty e^{-i\omega t}\, A(\omega,x_0)\, d\omega$$

$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^\infty e^{-i\omega t}\, A(\omega,x_0)\, d\omega = T(t,x_0) \quad .$$

Note the explicit use of the fact that $A(\omega,x_0) = 0$ for $\omega \leq 0$. Thus if we restrict attention to the domain of time amplitude functions (this always happens when we work in a time domain) the required orthogonality holds.

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[1] Allcock, G.R. 1969: ANN. Phys. (N.Y.), 53,253.

The operator $\frac{1}{2\pi}\int_0^\infty e^{i\omega(t'-t)}\,d\omega$ is a Hermitian operator on functions of t' since if one interchanges t' and t and takes complex conjugates the result is the same. The transpose (or conjugate) operator $\frac{1}{2\pi}\int_0^\infty e^{-i\omega(t'-t)}\,d\omega$ transforms $T(t',x_0)$ to zero.

The Space of Time Amplitude Functions and its Conjugate

A function of t on the range $-\infty$ to ∞ which can be expanded in terms of $e^{-i\omega t}$ for positive ω only is said to lie in the domain of time amplitude functions. The conjugate space of time amplitude functions consists of those which can be expanded in terms of $e^{i\omega t}$ for positive ω .

If $T(t)$ lies in the domain D of time amplitude functions, $T^*(t)$ is in the conjugate domain D^* . Also $t\,T(t)$ and $\frac{\partial T}{\partial t}(t)$ are in D . To see this let $T(t) = \frac{1}{\sqrt{2\pi}}\int_0^\infty A(\omega)\,e^{-i\omega t}\,d\omega$. Then

$$t\,T(t) = \frac{1}{\sqrt{2\pi}}\int_0^\infty i\,A(\omega)\,\frac{\partial}{\partial\omega}\left(e^{-i\omega t}\right)d\omega$$

$$= \frac{1}{\sqrt{2\pi}}\left[i\,A(\omega)\,e^{-i\omega t}\right]_0^\infty - \frac{1}{\sqrt{2\pi}}\int_0^\infty i\,\frac{\partial}{\partial\omega}\left[A(\omega)\right]e^{-i\omega t}\,d\omega$$

$$= \frac{1}{\sqrt{2\pi}}\int_0^\infty -i\,\frac{\partial}{\partial\omega}\left[A(\omega)\right]e^{-i\omega t}\,d\omega$$

for $A(\omega)$ zero at $\omega = 0$ and ∞ . Also $\frac{\partial}{\partial t} T(t) = \frac{1}{\sqrt{2\pi}} \int_0^\infty (-i\omega A(\omega))$ $e^{-i\omega t}\, d\omega \in T$, in fact $i \frac{\partial}{\partial t} T(t) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \omega\, A(\omega)\, e^{-i\omega t}\, d\omega$. This illustrates the operator equivalence $i \frac{\partial}{\partial t} \sim \omega$ and $t \sim - i \frac{\partial}{\partial \omega}$. Since $T(t) \in D$ we see $t\, T^*(t) \in D^*$ and $\frac{\partial T^*}{\partial t}(t) \in D^*$. Let us return to a calculation done earlier, and explicitly examine the missing steps in order to show how these results apply. When we showed that $f_{\vec{r}_0(t-t_0)}(\vec{r})$ was an eigenfunction of $T_{\vec{r}_0, t_0}$ with eigenvalue t we claimed

$$\int_{\text{space}} T_{\vec{r}_0, t_0}(\vec{r}', \vec{r})\, f_{\vec{r}_0(t-t_0)}(\vec{r})\, d\vec{r}$$

$$= \int_{\text{space}} f_{\vec{r}_0(t-t_0)}(\vec{r})\, d\vec{r} \int_{-\infty}^{\infty} t'\, f_{\vec{r}_0(t'-t_0)}(\vec{r}')\, f^*_{\vec{r}_0(t'-t_0)}(\vec{r})\, dt'$$

$$= \int_{-\infty}^{\infty} t'\, f_{\vec{r}_0(t'-t_0)}(\vec{r}')\, \delta(t-t')\, dt' = t\, f_{\vec{r}_0(t-t_0)}(\vec{r}') \ .$$

Is the insertion of $\delta(t-t')$ justified? In the light of new evidence, we can show that it is. What we claimed to be $\delta(t-t')$ was actually

$$\int_{\text{space}} f_{\vec{r}_0(t-t_0)}(\vec{r})\, f^*_{\vec{r}_0(t'-t_0)}(\vec{r})\, d\vec{r} = \frac{1}{2\pi} \int_0^\infty e^{i\omega(t-t')}\, d\omega$$

as we showed earlier. The order $t-t'$ (and not $t'-t$) is of great importance. Substituting in the other integral we have

$$\int_{-\infty}^{\infty} t'\, f_{\vec{r}_0(t'-t_0)}(\vec{r}')\, dt' \left(\frac{1}{2\pi} \int_0^\infty e^{i\omega(t-t')}\, d\omega \right) \ .$$

In order for this integral over ω to behave like $\delta(t-t')$ we require that t' $f_{\vec{r}_0(t'-t_0)}(\vec{r}') \in D^*_{t'}$ the conjugate space of time amplitude functions of t' . This is true if $f_{\vec{r}_0(t'-t_0)}(\vec{r}') \in D^*_{t'}$. But recall that $f_{\vec{r}_0(t'-t_0)}(\vec{r}') = \frac{1}{\sqrt{2\pi}} \int_0^\infty \psi_{\omega,\vec{r}_0}(\vec{r}')\, e^{i\omega(t'-t_0)}\, d\omega$ from which we see immediately that $f_{\vec{r}_0(t'-t_0)}(\vec{r}') \in D^*_{t'}$, since the expansion is in terms of $e^{i\omega t'}$ for positive ω .

Observe that if $T(t) \in D_t$ and $T(t)$ is a real valued function of t , then $T(t) \equiv 0$ for all t .

CHAPTER XI

THE TIME DELAY OPERATOR

In three dimensional space we consider the Hamiltonian for a central potential $H = -\frac{\hbar^2}{2M}\nabla^2_{\vec{r}} + V(r)$ where $r = |\vec{r}|$. We note that H , L^2 , L_z are mutually commuting Hermitian operators with common eigenfunctions $R_{\omega\ell}(r)\, Y^m_\ell(\theta,\phi) = \psi_{\omega\ell m}(\vec{r})$ where $H\psi_{\omega\ell m} = \hbar\omega\psi_{\omega\ell m}$, $L^2\psi_{\omega\ell m} = \ell(\ell+1)\hbar^2\, \psi_{\omega\ell m}$ and $L_z\, \psi_{\omega\ell m} = m\hbar\, \psi_{\omega\ell m}$ for m and ℓ integers, $\ell \geq 0$, $|m| \leq \ell$ and $\omega > 0$ is real. We assume that the potential $V(r)$ is local so that all $\omega > 0$ are possible.

Classically, the time delay for a potential of range A is given by

$$\partial t = 2\int_{r_{min}}^{A} \frac{ds}{\sqrt{v_0^2\left(1 - \frac{b^2}{s^2}\right) - \frac{2}{M}V(s)}} - 2\int_{b}^{A} \frac{ds}{\sqrt{v_0^2\left(1 - \frac{b^2}{s^2}\right)}} \ .$$

Also classically $H = \frac{p_r^2}{2M} + \frac{L^2}{2Mr^2} + V(r) = \frac{1}{2}Mv_0^2$ and $L^2 = M^2b^2\, v_0^2$. Thus we can write

$$\partial t = \sqrt{2M}\int_{r_{min}}^{A} \frac{ds}{\sqrt{H - \frac{L^2}{2Ms^2} - V(s)}} - \sqrt{2M}\int_{b}^{A} \frac{ds}{\sqrt{H - \frac{L^2}{2Ms^2}}} \ .$$

The lower limits r_{min} and b of integration cause the denominators in the respective integrands to be zero.

To make an operator out of ∂t we replace H and L^2 by the respective operators. Since H and L^2 have common eigenfunctions $\psi_{\omega\ell m}$ we can see that $\psi_{\omega\ell m}$ are eigenfunctions of ∂t with eigenvalues

$$\lambda_{\omega\ell} = \sqrt{2M}\int_{r_{\min}(\omega,\ell)}^{A} \frac{ds}{\sqrt{\hbar\omega - \frac{\ell(\ell+1)\hbar^2}{2Ms^2} - V(s)}} - \sqrt{2M}\int_{b(\omega,\ell)}^{A} \frac{ds}{\sqrt{\hbar\omega - \frac{\ell(\ell+1)\hbar^2}{2Ms^2}}} .$$

The lower limits of integration in each case are selected to make the denominator zero. The eigenfunction equation $\partial t\, \psi_{\omega\ell m} = \lambda_{\omega\ell}\, \psi_{\omega\ell m}$ completely determines the operator ∂t since $\psi_{\omega\ell m}$ are a complete set.

Observe that H and L^2 are classical constants of the motion and quantum mechanically compatible observables. Suppose we make measurements of a state and find that the energy is always $\hbar\omega$ and the square of angular momentum is always $\ell(\ell+1)\hbar^2$. Classically, the parameters b and v_0 are specified and so ∂t is uniquely determined. For such a state any measurement of ∂t always yields the fixed value $\lambda_{\omega\ell}$. Thus this state is also an eigenstate of the time delay operator and has eigenvalue $\lambda_{\omega\ell}$.

Integrating the final term we can simplify the expression for $\lambda_{\omega\ell}$ as

$$\lambda_{\omega\ell} = \sqrt{2M}\int_{r_{\min}(\omega,\ell)}^{A} \frac{ds}{\sqrt{\hbar\omega - \frac{\ell(\ell+1)}{2Ms^2} - V(s)}} - \sqrt{\frac{2MA^2}{\hbar\omega} - \frac{\ell(\ell+1)}{\omega^2}} .$$

We observe that the time delay is simply a function of the two constants H and L^2 of the motion in the classical case, i.e.

$$\begin{aligned} \partial t &= f(H,L^2) \\ &= \sqrt{2M}\int_{r_{\min}}^{A} \frac{ds}{\sqrt{H - \frac{L^2}{2Ms^2} - V(s)}} - \sqrt{2M}\int_{b}^{A} \frac{ds}{\sqrt{H - \frac{L^2}{2Ms^2}}} \\ &= \sqrt{2M}\int_{r_{\min}}^{A} \frac{ds}{\sqrt{H_0 - \frac{L^2}{2Ms^2}}} - \sqrt{2M}\int_{b}^{A} \frac{ds}{\sqrt{H_0 + V(s) - \frac{L^2}{2Ms^2}}} \;. \end{aligned}$$

Since H_0 is not a constant, but a function of s we cannot make an operator substitution for H_0 and L^2, even though there is a set of eigenfunctions of H_0 and L^2. Observe that

$$\begin{aligned} \partial t\, \psi_{\omega \ell m} &= f(H,L^2)\psi_{\omega \ell m} = f(\hbar\omega, \ell(\ell+1)\hbar^2)\psi_{\omega \ell m} \\ &= \lambda_{\omega \ell}\, \psi_{\omega \ell m} \;. \end{aligned}$$

The time delay operator ∂t commute with H and L^2 for a central potential $V(r)$. This follows from the fact that H, L^2 and ∂t all share the same eigenfunctions $\psi_{\omega \ell m}$. Moreover all the eigenvalues of these operators are degenerate in m.

Time Delay in Scattering

We must enlarge on the concept of time delay if it is to be properly applied to the theory of scattering. In addition to our time delay operator ∂t we introduce the scattering angle operator Θ_s. Recall that classically

$$\Theta_s = \pi - 2bv_0 \int_{r_{min}}^{\infty} \frac{dr}{r^2\sqrt{v_0^2[1 - \frac{b^2}{r^2}] - \frac{2}{m} V(r)}}$$

$$= \pi - \sqrt{\frac{2}{M}}\, L \int_{r_{min}}^{\infty} \frac{dr}{r^2\sqrt{H - \frac{L^2}{2Mr^2} - V(r)}} \quad .$$

r_{min} is selected so as to make the square root zero. Observe that Θ_s is uniquely determined as a function of the parameters H and L^2 which are classical constants of the motion and quantum mechanically compatible observables. Thus the operator Θ_s satisfies the eigenvalue equation $\Theta_s \psi_{\omega\ell m} = \Theta_{\omega\ell} \psi_{\omega\ell m}$ where

$$\Theta_{\omega\ell} = \pi - \sqrt{\frac{2}{M}} \sqrt{\ell(\ell+1)\hbar} \int_{r_{min}(\omega,\ell)}^{\infty} \frac{dr}{r^2\sqrt{\hbar\omega - \frac{\ell(\ell+1)\hbar^2}{2Mr^2} - V(r)}} \quad .$$

Observe that the eigenvalues $\Theta_{\omega\ell}$ are scattering angle values and are not directly related to the observed angular position of detection, since the direction of incidence in quantum mechanics may not be precisely known. Thus Θ_s is not an operator whose eigenvalues measure the angular component of the point of detection.

The operator ∂t can be used to measure time delay. If we measure $<\partial t>$ on a particular wave packet for instance, we get a single average time delay value, but we do not obtain time delay expectation at a given scattering angle.

The Time Delay Operator in One Dimension

Let us consider the time delay operator in one dimension. We will find it is Hermitian but not always self-adjoint. In fact, it is possible to determine for specific types of potential exactly what the domain of the time delay operator is.

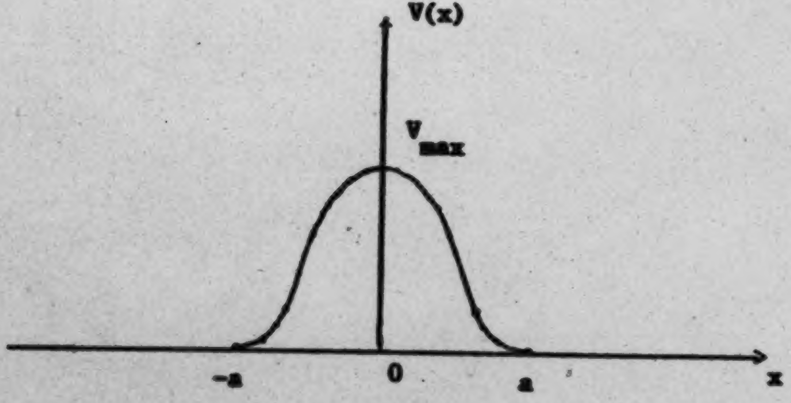

Figure 18

Positive Potential

Case 1: $V(x) \geq 0$, $V(x) = 0$ for $|x| > a$. The Hamiltonian $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$ has every eigenfunctions $\psi_\omega(x)$ with $H\,\psi_\omega(x) = \hbar\omega\psi_\omega(x)$, $\psi_\omega(x) = c(\sqrt{\frac{2m\omega}{\hbar}})\sqrt[4]{\frac{m}{2\hbar\omega}}\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\, x}$ for $x > a$, where $c(k)$ is the transmission coefficient for the momentum transformation kernel. In this way, $\psi_\omega(x)$ is normalized to satisfy $\int_{-\infty}^{\infty} \psi_\omega^*(x)\, \psi_{\omega'}(x)\, dx = \delta(\omega-\omega')$ for $\omega, \omega' > 0$, and $\psi_\omega(x)$ respresent a moneonergetic "wave packet" with energy $\hbar\omega$ which moves in the positive direction only for $x > a$.

The $\psi_\omega(x)$, $\omega > 0$ form a complete normalized set of functions for expanding other functions in terms of in this time domain. A general wave packet which initially approaches the potential from negative x can be expanded as

$$\psi(x,t) = \int_0^\infty A(\omega)\, \psi_\omega(x)\, e^{-i\omega t} \quad .$$

We can define a time delay operator on the Hilbert space spanned by $\psi_\omega(x)$ by specifying precisely how it operates on each $\psi_\omega(x)$. We insist that $\psi_\omega(x)$ be an eigenfunction of the operator ∂t with eigenvalue λ_ω , that is $\partial t(\psi_\omega(x)) = \lambda_\omega \psi_\omega(x)$, where λ_ω is the classical time delay for a particle with intial energy $\hbar\omega$ to pass over the potential. Thus

$$\lambda_\omega = \sqrt{\frac{m}{2}}\ [\int_{-a}^{a} \frac{dx}{\sqrt{\hbar\omega - V(x)}} - \frac{2a}{\sqrt{\hbar\omega}}] \quad .$$

Let $V_{max} > 0$ be the maximum value achieved by the potential $V(x)$. Then λ_ω is only defined for $\hbar\omega > V_{max}$. This means that the domain of the time delay operator is that subspace of the Hilbert space spanned by $\psi_\omega(x)$ for $\omega > \frac{V_{max}}{\hbar}$. It is a Hermitian operator, since its eigenvalues λ_ω are real but it is not self adjoint, since not all $\psi_\omega(x)$ are in the domain of ∂t.

Case 2: $V(x) \leq 0$ always, $V(x) = 0$ for $|x| > a$.

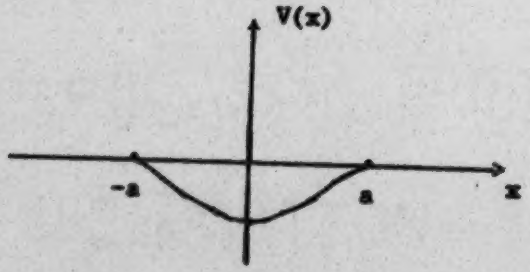

Figure 19

Negative Potential

$\psi_\omega(x)$ is defined as in case 1. Instead of a time delay we leave a time advance in this case, since λ_ω defined above is negative. In this case $\partial t(\psi_\omega(x)) = \lambda_\omega \psi_\omega(x)$ defines ∂t on $\psi_\omega(x)$ for all $\omega > 0$. $\psi_\omega(x)$ span a complete Hilbert space as long as the finite range attractive potential is not strong enough to allow the existence of one or more bound states (always finite in number) with discrete negative energy levels. If bound states exist, ∂t is only defined on that subspace of the Hilbert space generated by the positive energy eigenfunctions $\psi_\omega(x)$ for $\omega > 0$. Any function in the domain of ∂t is orthogonal to every bound state. No time delay concept is associated with bound states.

If we take $V(x) = V_0\,\delta(x)$ where $V_0 > 0$ one can easily see that no time delay operator ∂t can be defined in this way since the delta function barrier cannot be penetrated classically and the integral for λ_ω does not make sense. Thus the domain of ∂t is zero. If we take $V_0 < 0$, ∂t has a complete domain of functions $\psi_\omega(x)$, (excluding the bound states since one exists), but the value of λ_ω is zero for each ω , so ∂t is the zero operator. It becomes clear that our concept of what time delay actually is turns out to be less than ideal. The operators we have defined for ∂t are known as classical time delay operators. In constructing them we have taken classical formulas for time delay in terms of energy in one dimension, and time delay in terms of energy and angular momentum in three dimensions, namely

$$\partial t = \sqrt{\frac{m}{2}}\,\left[\int_{-a}^{a} \frac{dx}{\sqrt{E-V(x)}} - \frac{2a}{\sqrt{E}}\right] ,$$

and

$$\partial t = \sqrt{2m}\left[\int_{r_{\min}}^{A} \frac{ds}{\sqrt{E - \frac{L^2}{2ms^2} - V(s)}} - \int_{b}^{A} \frac{ds}{\sqrt{E - \frac{L^2}{2ms^2}}}\right]$$

and assumed that these were definitions for the actual concept of what time delay means. In fact time delay in the sense we would like to think of it as, is not a simple function of energy or energy and angular momentum. What we have constructed is an operator for the quantity defined above in the integrals which is classical time delay. Therefore this operator ∂t should rightfully be called the classical time delay operator. We saw that in one dimension for a slowly varying local potential, with particle energy much greater than the maximum potential height, the W.K.B. approximation told us that the expected quantum time delay was the classical time delay defined as in the above integral. First of all, we recall a calculation done earlier to determine the commutator of a time delay operator with the Hamiltonian H including kinetic energy and potential.

The result was $[H,\tau_d] = -[V,\tau_f]$. In our calculations with $\tau_d = \partial t$, we observe that τ_d and H have the same eigenfunctions, and so $[H,\tau_d] = 0$. In general, there is no reason to suspect why the potential $V(x)$ should commute with τ_f a free particle time of arrival operator. This indicates that the classical time delay operator ∂t is not the same as τ_d the time delay concept, obtained by considering the difference of two time of arrival operators, one with the Hamiltonian including the potential and one for the free particle.

A General Discussion of the Time Delay Operator

Suppose we consider a typical scattering problem in which interaction of the particle with the potential is limited to a finite time interval. Let the wavefunction be described by

$$\psi(\vec{r},t) = \int_0^\infty A(\omega,\vec{r}_0)\, \psi_{\omega,\vec{r}_0}(\vec{r})\, e^{-i\omega t}\, d\omega \ .$$

$\psi(\vec{r},t)$ remains in the full Hamiltonian time domain D spanned by the functions $\psi_{\omega,\vec{r}_0}(\vec{r})$ as functions of $\vec{r}$ for all time t . Initially $\psi(\vec{r},t)$ corresponded with the free wave packet $\psi_1(\vec{r},t)$. $\psi_1(\vec{r},t)$ can be expanded in terms of the free energy eigenfunctions as

$$\psi_1(\vec{r},t) = \int_0^\infty A^f(\omega,\vec{r}_0)\, \psi^f_{\omega,\vec{r}_0}(\vec{r})\, e^{-i\omega t}\, d\omega$$

where $\psi^f_{\omega,\vec{r}_0}(\vec{r})$ satisfy

$$-\frac{\hbar^2}{2m} \nabla^2_{\vec{r}}\, \psi^f_{\omega,\vec{r}_0}(\vec{r}) = \hbar\omega\, \psi^f_{\omega,\vec{r}_0}(\vec{r})$$

so each $\psi^f_{\omega,\vec{r}_0}(\vec{r})$ is a superposition of the type

$$\psi^f_\omega(\vec{r}) = \int_{\hat{k}} B_\omega(\hat{k})\, e^{i\sqrt{\frac{2m\omega}{\hbar}}\,\hat{k}\cdot\vec{r}}\, d\Omega_{\hat{k}} \quad .$$

$\psi_1(\vec{r},t)$ remains in the free Hamiltonian time domain D^f spanned by $\psi^f_{\omega,\vec{r}_0}(\vec{r})$ for all time t. This time domain is a Hilbert subspace of functions of the vector variable $\vec{r}$. Since $\psi^f_{\omega,\vec{r}_0}(\vec{r})$ is a multiple of $\psi^f_{\omega,\vec{r}_1}(\vec{r})$ by a complex number of modulus 1, the time domain D^f is independent of what $\vec{r}_0$ is chosen. In a similar way, D is independent of the choice of $\vec{r}_0$ in $\psi_{\omega,\vec{r}_0}(\vec{r})$.

We can construct time of arrival operators $T_{\vec{r}_0,t_0}$ on D and $T^f_{\vec{r}_0,t_0}$ on D^f defined by

$$T_{\vec{r}_0,t_0}[\psi_{\omega,\vec{r}_0}(\vec{r})] = (t_0 + i\frac{\partial}{\partial\omega})[\psi_{\omega,\vec{r}_0}(\vec{r})] \quad ,$$

$$T^f_{\vec{r}_0,t_0}[\psi^f_{\omega,\vec{r}_0}(\vec{r})] = (t_0 + i\frac{\partial}{\partial\omega})[\psi^f_{\omega,\vec{r}_0}(\vec{r})] \quad .$$

$\tau_{\vec{r}_0,t_0}$ and $\tau^f_{\vec{r}_0,t_0}$ are operators on functions of position $\vec{r}$. Observe

$\int_{\text{space}} \psi^*(r,t_0)\tau_{\vec{r}_0,t_0}\,\psi(\vec{r},t_0)d^3\vec{r} =$ the expected time of arrival for a particle at point $\vec{r}_0$ in full Hamiltonian. This integral is independent of t_0.

$\int_{\text{space}} \psi_1^*(\vec{r},t_0)\tau^f_{\vec{r}_0,t_0}\psi_1(\vec{r},t_0)d^3\vec{r} =$ the expected time of arrival for a particle at point $\vec{r}_0$ in the free Hamiltonian described by $\psi_1(r,t)$. This integral is independent of t_0.

The time delay operator is $\tau_{\vec{r}_0,t_0} - \tau^f_{\vec{r}_0,t_0}$ for measuring time delay at $\vec{r}_0$. It operates on a wavefunction at time t_0 which must be a time before the scattering interaction. At that time $\psi(\vec{r},t_0) = \psi_1(\vec{r},t_0)$ and this wave packet is contained in the intersection $D \cap D^f$ of time domains since $\psi \in D$ and $\psi_1 \in D^f$ for all times.

What is the expected value of this time delay operator $\tau^d_{\vec{r}_0,t_0}$ given by $\tau^d_{\vec{r}_0,t_0} = \tau_{\vec{r}_0,t_0} - \tau^f_{\vec{r}_0,t_0}$ on the wave packet $\psi_1(\vec{r},t_0) = \psi(\vec{r},t_0)$ at this time t_0 before the scattering? It is given by

$$\langle\tau^d_{\vec{r}_0,t_0}\rangle_{t_0} = \int_{\text{space}} \psi_1^*(\vec{r},t_0)\;\tau^d_{\vec{r}_0,t_0}\;\psi_1(\vec{r},t_0)\;d^3\vec{r}$$

$$= \int_{\text{space}} \psi^*(\vec{r},t_0)\tau_{\vec{r}_0,t_0}\psi(\vec{r},t_0)d^3\vec{r} - \int_{\text{space}} \psi_1^*(\vec{r},t_0)\tau^f_{\vec{r}_0,t_0}\psi_1(\vec{r},t_0)d^3\vec{r}$$

$$= \begin{bmatrix} \text{Expected time of arrival} \\ \text{at } \vec{r}_0 \text{ for full Hamiltonian} \end{bmatrix} - \begin{bmatrix} \text{Expected time of arrival} \\ \text{at } \vec{r}_0 \text{ for free Hamiltonian} \end{bmatrix}$$

$$= \text{Time delay due to potential observed at } \vec{r}_0 \; .$$

This time delay concept is different from the classical "impact parameter time delay" we discussed in the three dimensional case, since there we measured the time of arrival with and without potential at different points equidistant from the origin and separated by the scattering angle, while in this new time delay concept, the same $\vec{r}_0$ is used for both free particle and potential time of arrival.

It is a good exercise in manipulating integrals to start with

$$\langle t\rangle_{\vec{r}_0} = \int_{\text{space}} \psi^*(\vec{r},t_0)\, \tau_{\vec{r}_0,t_0}\, \psi(\vec{r},t_0)\, d^3\vec{r} \quad ,$$

$$\psi(\vec{r},t_0) = \int_0^\infty A(\omega,\vec{r}_0)\, \psi_{\omega,\vec{r}_0}(\vec{r})\, e^{-i\omega t_0}\, d\omega \quad ,$$

and

$$\tau_{\vec{r}_0,t_0}\psi_{\omega,\vec{r}_0}(\vec{r}) = \left(t_0 + i\frac{\partial}{\partial\omega}\right) \psi_{\omega,\vec{r}_0}(\vec{r})$$

and show that

$$\langle t\rangle_{\vec{r}_0} = \int_0^\infty A^*(\omega,\vec{r}_0)\left[-i\frac{\partial}{\partial\omega}\right] A(\omega,\vec{r}_0)\, d\omega \quad .$$

To do this, one needs to use the orthogonality relation

$$\int_{\text{space}} \psi^{*}_{\bar{\omega},\vec{r}_0}(\vec{r})\, \psi_{\omega,\vec{r}_0}(\vec{r})\, d^3\vec{r} = \delta(\omega-\bar{\omega}) \quad .$$

CHAPTER XII

THE DEVELOPMENT OF TIME MEASUREMENT IN 3-DIMENSIONAL SCATTERING

We already know the result for the time dependence of a free particle in Cartesian coordinates for two and three dimensions. These results are:

$$\psi(\underline{x},t) = \frac{-im}{2\pi\hbar(t-t_0)} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi(\underline{\bar{x}},t_0)\ \exp\ (\frac{im(\underline{\bar{x}}-\underline{x})^2}{2\hbar(t-t_0)})d\underline{\bar{x}}$$

(for two dimensions $\underline{x} = (x_1,x_2)$), and

$$\psi(\underline{x},t) = \frac{-(1+i)}{4} (\frac{m}{\pi\hbar(t-t_0)})^{3/2} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi(\underline{\bar{x}},t_0)\exp\ (\frac{im(\underline{x}-\underline{\bar{x}})^2}{2\hbar(t-t_0)})d\underline{\bar{x}}$$

(for three dimensions $\underline{x} = (x_1,x_2,x_3)$).

We shall consider the time dependence of free particles in other coordinate systems, namely 2-dimensional polar coordinates (which can be extended to three-dimensional cylindrical coordinates) and 3-dimensional spherical coordinates. We shall be interested in both position and momentum wavefunctions.

Two Dimensional Polar Coordinates

In the coordinates $x = \rho \cos\phi$ and $y = \rho \sin\phi$ the equation $i\hbar \frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2})$ transforms into the new equation

$$i\hbar \frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}(\frac{\partial^2\psi}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial\psi}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\phi^2}).$$

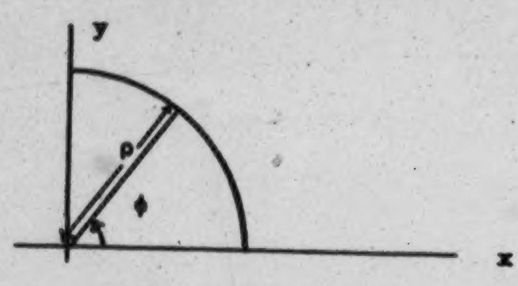

Figure 20 Polar Coordinates

In order to solve this equation for ψ we separate variables $\psi(\rho,\phi,t) = X(\rho,\phi)T(t)$. This means $i\hbar\,\frac{T'}{T} = \frac{-\hbar^2}{2m}\,\frac{\nabla^2 X}{X} = \frac{\hbar^2 k^2}{2m}$. Thus $T(t) = e^{-(i\hbar k^2 t/2m)}$ and X satisfies $\nabla^2 X + k^2 X = 0$, or $\frac{\partial^2 X}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial X}{\partial\rho} + \frac{1}{\rho^2}\,\frac{\partial^2 X}{\partial\phi^2} + k^2 X = 0$. We separate variables again by taking $X(\rho,\phi) = R(\rho)S(\phi)$. From this we get $\rho^2\,\frac{R''}{R} + \frac{\rho R'}{R} + \frac{S''}{S} + k^2\rho^2 = 0$. This implies $\frac{S''}{S} = -n^2$ a constant and $\rho^2 R'' + \rho R' + k^2\rho^2 R = n^2 R$. $\frac{S''}{S} = -n^2$ implies $S = e^{in\phi}$ and n must be an integer in order to satisfy the condition of single valueness. The equation $\rho^2 R'' + \rho R' + (k^2\rho^2 - n^2)R = 0$ is related to Bessel's equation, and the solution which is bounded at the origin is $J_{|n|}(k\rho)$. The separable solution is $J_{|n|}(k\rho)e^{in\phi}\,e^{-(i\hbar k^2 t/2m)}$. The general solution involves a superposition over k and a sum over n, that is

$$\psi(\rho,\phi,t) = \int_0^\infty \sum_{n=-\infty}^{\infty} A_n(k)J_{|n|}(k\rho)e^{in\phi}\,e^{-(i\hbar k^2 t/2m)}\,dk\,.$$

Thus evaluating at t_0 we get

$$\psi(\rho,\phi,t_0) = \int_0^\infty \sum_{n=-\infty}^{\infty} A_n(k)J_{|n|}(k\rho)e^{in\phi}\,e^{-(i\hbar k^2 t_0/2m)}\,dk\,.$$

The first thing to do is to obtain $A_n(k)$ in terms of $\psi(\rho,\phi,t_0)$. Multiply by $\frac{1}{2\pi}\,e^{-i\ell\phi}$ and integrate over ϕ between $-\pi$ and π to get

$$\frac{1}{2\pi}\int_{-\pi}^{\pi}\psi(\rho,\phi,t_0)e^{-i\ell\phi}\,d\phi = \int_0^\infty A_\ell(k)J_{|\ell|}(k\rho)e^{-i\hbar k^2 t_0/2m}\,dk\ .$$

Next of all, we use the Hankel transform representation of the delta function, namely $\delta(x-y) = \int_0^\infty tyJ_\nu(tx)J_\nu(ty)dt$ where $\nu \geq -\frac{1}{2}$ and $x,y > 0$. In order to use this, we multiply by $\bar{k}\rho J_{|\ell|}(\bar{k}\rho)$ and integrate over ρ to get

$$\frac{1}{2\pi}\int_{\phi=-\pi}^{\pi}\int_{\rho=0}^{\infty}\psi(\rho,\phi,t_0)\bar{k}\rho J_{|\ell|}(\bar{k}\rho)e^{-i\ell\phi}d\rho d\phi$$

$$= \int_0^\infty A_\ell(k)\delta(k-\bar{k})e^{-(i\hbar k^2 t_0/2m)}\,dk = A_\ell(\bar{k})e^{-(i\hbar\bar{k}^2 t_0/2m)}\ .$$

Thus we see that

$$A_\ell(\bar{k}) = \frac{1}{2\pi}\,e^{(i\hbar\bar{k}^2 t_0/2m)}\int_{\phi=-\pi}^{\pi}\int_{\rho=0}^{\infty}\psi(\rho,\phi,t_0)\bar{k}\rho J_{|\ell|}(\bar{k}\rho)e^{-i\ell\phi}d\rho d\phi\ .$$

We can substitute for $A_n(k)$ into the original expression for $\psi(\rho,\phi,t)$

$$A_n(k) = \frac{1}{2\pi}\,e^{(i\hbar k^2 t_0/2m)}\int_{\bar{\phi}=-\pi}^{\pi}\int_{\bar{\rho}=0}^{\infty}\psi(\bar{\rho},\bar{\phi},t_0)k\bar{\rho}J_{|n|}(k\bar{\rho})e^{-in\bar{\phi}}\,d\bar{\rho}d\bar{\phi}\ ,$$

and hence

$$\psi(\rho,\phi,t) = \int_{k=0}^{\infty}\sum_{n=-\infty}^{\infty}\int_{\bar{\phi}=-\pi}^{\pi}\int_{\bar{\rho}=0}^{\infty}$$

$$\frac{1}{2\pi}\,\psi(\bar{\rho},\bar{\phi},t_0)k\bar{\rho}J_{|n|}(k\bar{\rho})J_{|n|}(k\rho)e^{in(\phi-\bar{\phi})}\,e^{-(i\hbar k^2(t-t_0)/2m)}\,dkd\bar{\rho}d\bar{\phi}\ .$$

One could explicitly sum over n and integrate over k and obtain the time shift operator for the position wavefunction in polar coordinates.

Alternatively, let us consider the momentum wavefunction in polar coordinates. We denote it by $\phi(k,\beta,t)$, where $k = |\underline{k}|$ the magnitude of the momentum vector, and β is an angle specifying its direction, so that $k_1 = k\cos\beta$ and $k_2 = k\sin\beta$. ϕ satisfies the differential equation $i\hbar\frac{\partial\phi}{\partial t} = \frac{\hbar^2k^2}{2m}\phi$. Thus the time dependence of ϕ is very much simpler than that of ψ, namely

$$\phi(k,\beta,t) = \phi(k,\beta,t_0)\,e^{-(i\hbar k^2(t-t_0)/2m)} .$$

ψ is related to ϕ by means of Fourier transforms

$$\psi(\rho,\phi,t) = \frac{1}{2\pi}\int_{-\pi}^{\pi}\int_0^\infty \phi(k,\beta,t)e^{ik\rho\cos(\phi-\beta)}kdkd\beta ,$$

$$\phi(k,\beta,t) = \frac{1}{2\pi}\int_{-\pi}^{\pi}\int_0^\infty \psi(\rho,\phi,t)e^{-ik\rho\cos(\phi-\beta)}\rho d\rho d\phi .$$

In the case of a free particle in two-dimensional polar coordinates we see the great advantage of working with the momentum wavefunction instead of the position wavefunction.

The normalization conditions in polar coordinates are

$$\int_{-\pi}^{\pi}\int_0^\infty |\psi(\rho,\phi,t)|^2\,\rho d\rho d\phi = 1 = \int_{-\pi}^{\pi}\int_0^\infty |\phi(k,\beta,t)|^2\,kdkd\beta .$$

We can derive an alternative form for the time dependence of the position wavefunction using the above Fourier Transform relations.

$$\psi(\rho,\phi,t) = \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{0}^{\infty} \int_{-\pi}^{\pi} \int_{0}^{\infty} \psi(\bar{\rho},\bar{\phi},t_0) e^{-(i\hbar k^2(t-t_0)/2m)}$$

$$e^{ik[\rho\cos(\phi-\beta)-\bar{\rho}\cos(\bar{\phi}-\beta)]} \bar{\rho} k dk d\beta d\bar{\rho} d\bar{\phi} \quad .$$

The simplest expression for the time dependence of $\psi(\rho,\phi,t)$ is found by transforming the two dimensional cartesian integral into polar coordinates. Thus we have

$$\psi(\rho,\phi,t) = -\frac{im}{2\pi\hbar(t-t_0)} \int_{-\pi}^{\pi} \int_{0}^{\infty} \psi(\bar{\rho},\bar{\phi},t_0)$$

$$\exp\left(\frac{im[\rho^2+\bar{\rho}^2-2\rho\bar{\rho}\cos(\phi-\bar{\phi})]}{2\hbar(t-t_0)}\right) \bar{\rho}\, d\bar{\rho}\, d\bar{\phi} \quad .$$

This result can be extended to three dimensional cylindrical coordinates ρ, ϕ, z where we have

$$\psi(\rho,\phi,z,t) = -\frac{(1+i)}{4} \left(\frac{m}{\pi\hbar(t-t_0)}\right)^{3/2} \int_{-\infty}^{\infty} \int_{-\pi}^{\pi} \int_{0}^{\infty} \psi(\bar{\rho},\bar{\phi},\bar{z},t_0)$$

$$\exp\left(\frac{im[\rho^2+\bar{\rho}^2-2\rho\bar{\rho}\cos(\phi-\bar{\phi})+(z-\bar{z})^2]}{2\hbar(t-t_0)}\right) \bar{\rho}\, d\bar{z}\, d\bar{\rho}\, d\bar{\phi} \quad .$$

In spherical polar coordinates r, θ, ϕ with $x = r\cos\phi\sin\theta$, $y = r\sin\phi\sin\theta$, $z = r\cos\theta$ we have

$$\psi(r,\theta,\phi,t) = -\frac{(1+i)}{4} \left(\frac{m}{\pi\hbar(t-t_0)}\right)^{3/2} \int_{0}^{\infty} \int_{0}^{\pi} \int_{-\pi}^{\pi} \psi(\bar{r},\bar{\theta},\bar{\phi},t_0)$$

$$\exp\left(\frac{im[r^2+\bar{r}^2-2r\bar{r}\{\cos\theta\cos\bar{\theta}+\sin\theta\sin\bar{\theta}\cos(\phi-\bar{\phi})\}]}{2\hbar(t-t_0)}\right)$$

$$\bar{r}^2 \sin\bar{\theta}\, d\bar{r}\, d\bar{\theta}\, d\bar{\phi} \quad .$$

Separation of Variables in Spherical Coordinates

For a spherical coordinate system, let us look at the free particle equation $i\hbar \frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2\psi$. For $\psi(r,\theta,\phi,t)$ we have

$$\nabla^2\psi = \frac{1}{r^2 \sin\theta}\left[\frac{\partial}{\partial r}\left(r^2 \sin\theta \frac{\partial\psi}{\partial r}\right) + \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial\psi}{\partial\theta}\right) + \frac{\partial}{\partial\phi}\left(\frac{1}{\sin\theta}\frac{\partial\psi}{\partial\phi}\right)\right]$$

$$= \frac{\partial^2\psi}{\partial r^2} + \frac{2}{r}\frac{\partial\psi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2} + \frac{\cot\theta}{r^2}\frac{\partial\psi}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} \quad .$$

Since spherical polar coordinates lend themselves well to a central potential $V(r)$ which depends only on the distance from the origin, namely the positive scalar r, let us solve the energy eigenfunction equation $-\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\psi(\vec{r}) = E\psi(\vec{r})$, for some constant E. We write $\psi(\vec{r}) = R(r)T(\theta)B(\phi)$ as a trial separation and substitute into the above equation to get

$$-\frac{\hbar^2}{2M}R'' - \frac{\hbar^2}{Mr}R' + \left(\frac{\hbar^2\lambda}{2Mr^2} + V(r)\right)R = ER \quad ,$$

$$B'' + m^2 B = 0 \quad ,$$

$$\sin^2\theta T'' + \sin\theta\cos\theta\, T' + (\lambda\sin^2\theta - m^2)T = 0 \quad .$$

We can reformulate the θ equation by writing $T(\theta) = P(\cos\theta)$, in which case the function $P(\xi)$ satisfies

$$(1-\xi^2)P''(\xi) - 2\xi P'(\xi) + \left(\lambda - \frac{m^2}{1-\xi^2}\right)P(\xi) = 0 \quad .$$

This last equation is known as the associated Legendre equation. It turns out that the only physically acceptable solutions occur when $\lambda = \ell(\ell+1)$ where $\ell = 0,1,2,3,\ldots$ is an integer and m is an integer satisfying $|m| \leq \ell$. From the equation $B'' + m^2B = 0$ we see $B = e^{im\phi}$ and since ϕ is a periodic coordinate with period 2π, m must be an integer for single valuedness.

The associated Legendre functions are denoted by $P_\ell^m(\xi)$. The product $T(\theta)\,B(\phi) = P_\ell^m(\cos\theta)e^{im\phi}$ is known as a spherical harmonic and is denoted by $Y_\ell^m(\theta,\phi)$. These functions are assumed to be normalized so that

$$\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} Y_\ell^{m*}(\theta,\phi)Y_{\ell'}^{m'}(\theta,\phi)\sin\theta d\theta d\phi = \delta_{\ell\ell'}\delta_{mm'}$$

where of course $\ell = 0,1,2,3,\ldots$ and $m = -\ell,-\ell+1,\ldots,\ell-1,\ell$. This means Y_ℓ^m are orthonormal when integrated over solid angle. We can substitute $\lambda = \ell(\ell+1)$ in the radial equation to get

$$-\frac{\hbar^2}{2m}R''(r) - \frac{\hbar^2}{mr}R'(r) + \left(\frac{\hbar^2\ell(\ell+1)}{2mr^2} + V(r)\right)R(r) = \hbar\omega R(r) \quad .$$

Alternatively, we can write $U(r) = rR(r)$ and substitute into the radial equation above to obtain

$$-\frac{\hbar^2}{2m}U'' + \left[\frac{\hbar^2\ell(\ell+1)}{2mr^2} + V(r)\right]U(r) = \hbar\omega U(r)$$

which is a Schrödinger equation for the potential $\frac{\hbar^2\ell(\ell+1)}{2mr^2} + V(r)$

defined for the range of positive r. Suppose $V(r) = 0$ for $r > a$. The equation satisfied by $U(r)$ for $r > a$ is

$$-\frac{\hbar^2 U''}{2m} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} U(r) = \hbar\omega U(r) \quad \text{for } r > a \text{ , or}$$

$$-U'' + \frac{\ell(\ell+1)U}{r^2} = K^2 U(r) \quad \text{where} \quad \omega = \frac{\hbar k^2}{2m}.$$ The equation

$U''(r) + [k^2 - \frac{\ell(\ell+1)}{r^2}]\, U(r) = 0$ has solutions asymptotic to e^{ikr} or e^{-ikr} for large r, and so $R(r)$ is asymptotic to a linear combination of $\frac{e^{ikr}}{r}$ (outgoing waves) and $\frac{e^{-ikr}}{r}$ (incoming waves). For s waves ($\ell = 0$), these asymptotic forms are exact solutions.

The radial wave functions $R_{\omega,\ell}(r)$ which are defined for $\omega > 0$, $r > 0$ continuous, and $\ell = 0,1,2,3,\ldots$ discrete can be described for $r > a$ by spherical Bessel, Neumann or Hankel functions. The solutions are

$$j_\ell(kr) = j_\ell\left(\sqrt{\frac{2m\omega}{\hbar}}\, r\right) \quad \text{and} \quad n_\ell(kr)$$

or

$$h_\ell^{(1)}(kr) \quad \text{and} \quad h_\ell^{(2)}(kr) \quad .$$

j_ℓ and n_ℓ form 2 linearly independent solutions, and $h_\ell^{(1)}$ and $h_\ell^{(2)}$ form another set of 2 linearly independent solutions. There exact definitions are not important and will not be given here. The solution $j_\ell(kr)$ is regular at $r = 0$, and all others are unbounded at $r = 0$. Since we are only concerned with these solutions for $r > a$, the behavior at $r = 0$ is unimportant. The relation between the two solution sets is

$$j_\ell(z) = \frac{1}{2}[h_\ell^{(1)}(z)+h_\ell^{(2)}(z)] , \qquad n_\ell(z) = \frac{1}{2i}[h_\ell^{(1)}(z)-h_\ell^{(2)}(z)] .$$

The results of greatest interest to us are the asymptotic forms of $h_\ell^{(1)}(kr)$ and $h_\ell^{(2)}(kr)$. These asymptotes are

$$h_\ell^{(1)}(kr) \sim \frac{1}{kr} \exp(i[kr-(\ell+1)\frac{\pi}{2}]) ,$$

$$h_\ell^{(2)}(kr) \sim \frac{1}{kr} \exp(-i[kr-(\ell+1)\frac{\pi}{2}]) .$$

Similar expressions for $j_\ell(kr)$ and $n_\ell(kr)$ are

$$j_\ell(kr) \sim \frac{1}{kr} \cos\ (kr-(\ell+1)\frac{\pi}{2}) , \qquad n_\ell(kr) \sim \frac{1}{kr} \sin\ (kr-(\ell+1)\frac{\pi}{2}) .$$

In addition, plane waves moving in the z direction with momentum k can be expanded in terms of spherical outgoing and incoming waves

$$e^{ikz} = \sum_{\ell=0}^{\infty} (2\ell+1)i^\ell j_\ell(kr)P_\ell(\cos\theta) ,$$

$$= e^{ikr\cos\theta} .$$

These waves are independent of ϕ and so the quantum number m is zero. This simplification results from choosing plane waves propagating in the z direction.

From this we can see that $j_\ell(\rho) = \frac{1}{2i^\ell}\int_{-1}^{1} e^{i\rho s} P_\ell(s)ds$

$P_\ell(s)$ are the Legendre Polynomials, a form of the associated Legendre functions for $m = 0$.

ℓ is called the quantum number for total angular momentum, an m is the quantum number for z component of angular momentum. $Y_\ell^m(\theta,\phi)$ is an eigenfunction of L^2 and L_z satisfying

$$L^2 Y_\ell^m(\theta,\phi) = \ell(\ell+1)\hbar^2 Y_\ell^m(\theta,\phi) \qquad \text{and}$$

$$L_z Y_\ell^m(\theta,\phi) = -i\hbar \frac{\partial}{\partial\phi} Y_\ell^m(\theta,\phi) = m\hbar Y_\ell^m(\theta,\phi) \quad .$$

Observe that $Y_\ell^0(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta)$, independent of ϕ. The energy eigenfunctions can be expanded as

$$\psi_\omega(\vec{r}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell m}(\omega) R_{\omega\ell}(r) Y_\ell^m(\theta,\phi) \quad .$$

For scattering of a plane wave, only $m = 0$ contributes

$$\psi_\omega(\vec{r}) = \sum_{\ell=0}^{\infty} a_\ell(\omega) R_{\omega\ell}(r) \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta) \ , \quad \text{or}$$

$$\psi_\omega(\vec{r}) = \sum_{\ell=0}^{\infty} b_\ell(\omega) R_{\omega\ell}(r) P_\ell(\cos\theta) \ .$$

The eigenfunction $\psi_\omega(\vec{r})$ consists of a plane wave plus something asymptotic to an outgoing wave. Thus for $r = |\vec{r}|$ large, yet subject to the inequalities

$$|x|, |y| << \frac{1}{2}\sqrt{\frac{\hbar}{m\omega\epsilon}} \qquad \text{and} \qquad |z| \ll \frac{1}{\epsilon}\sqrt{\frac{\hbar}{2m\omega}}$$

we have $\psi_\omega(\vec{r}) \sim \frac{1}{2\pi}\sqrt{\frac{m\varepsilon}{\hbar}}\; k^{1/2}\,(e^{ikz} + f_k(\theta)\,\frac{e^{ikr}}{r})$ where $\omega = \frac{\hbar k^2}{2m}$ and $k > 0$.

e^{ikz} can be expressed in outgoing and incoming waves as

$$\begin{aligned}
e^{ikz} &= \frac{1}{2}\sum_{\ell=0}^{\infty} (2\ell+1)\, i^\ell h_\ell^{(1)}(kr) P_\ell(\cos\theta) + \frac{1}{2}\sum_{\ell=0}^{\infty} (2\ell+1)\, i^\ell h_\ell^{(2)} P_\ell(\cos\theta), \\
&\sim \frac{1}{2}\sum_{\ell=0}^{\infty} (2\ell+1)\,\frac{i^\ell}{k}\, e^{-i(\ell+1)\pi/2}\,\frac{e^{ikr}}{r}\,P_\ell(\cos\theta) \\
&\qquad + \frac{1}{2}\sum_{\ell=0}^{\infty} (2\ell+1)\,\frac{i^\ell}{k}\, e^{i(\ell+1)\pi/2}\,\frac{e^{-ikr}}{r}\,P_\ell(\cos\theta), \\
&\sim -\frac{i}{2k}\,\frac{e^{ikr}}{r}\sum_{\ell=0}^{\infty} (2\ell+1)P_\ell(\cos\theta) + \frac{i}{2k}\,\frac{e^{-ikr}}{r}\sum_{\ell=0}^{\infty} (-1)^\ell(2\ell+1)P_\ell(\cos\theta) .
\end{aligned}$$

Let the scattering amplitude $f_k(\theta)$ be expanded as

$f_k(\theta) = \sum_{\ell=0}^{\infty} \lambda_\ell(k) P_\ell(\cos\theta)$. From this we obtain the asymptotic form for $\psi_\omega(\vec{r})$ as

$$\begin{aligned}
\psi_\omega(\vec{r}) \sim \frac{1}{2\pi}\sqrt{\frac{m\varepsilon}{\hbar}}\, k^{1/2}\, \{ &\frac{e^{ikr}}{r}\sum_{\ell=0}^{\infty} [\lambda_\ell(k) - \frac{i}{2k}(2\ell+1)]P_\ell(\cos\theta) \\
&+ \frac{e^{-ikr}}{r}\,\frac{i}{2k}\sum_{\ell=0}^{\infty} (-1)^\ell(2\ell+1)P_\ell(\cos\theta)\} .
\end{aligned}$$

On the other hand we know that $\psi_\omega(\vec{r}) = \sum_{\ell=0}^{\infty} b_\ell(\omega) R_{\omega,\ell}(r) P_\ell(\cos\theta)$.

For $r > a$, $R_{\omega,\ell}(r)$ can be expressed in the form

$$R_{\omega,\ell}(r) = (1+\alpha_\ell(\omega))h_\ell^{(1)}(\sqrt{\frac{2m\omega}{\hbar}}\ r) + h_\ell^{(2)}(\sqrt{\frac{2m\omega}{\hbar}}\ r) \quad ,$$

where $\alpha_\ell(\omega)$ is a function characterizing the potential $V(r)$. For example, if $V(r) \equiv 0$ then $\alpha_\ell(\omega) \equiv 0$ in order that $R_{\omega,\ell}(r)$ be regular at $r = 0$. In a sense, the information provided by $\alpha_\ell(\omega)$ about $V(r)$ is analogous to that provided by the momentum transformation kernel in one dimension.

For large r we can write an asymptotic expression for $R_{\omega,\ell}(r)$

$$R_{\omega,\ell}(r) \sim \frac{(1+\alpha_\ell(\omega))}{k}\ e^{-i(\ell+1)\frac{\pi}{2}}\ \frac{e^{ikr}}{r} + \frac{1}{k}\ e^{i(\ell+1)\frac{\pi}{2}}\ \frac{e^{-ikr}}{r} \quad .$$

Substituting into the expression for $\psi_\omega(\vec{r})$ we get the asymptotic form

$$\psi_\omega(\vec{r}) \sim [\sum_{\ell=0}^{\infty} b_\ell(\omega)(-i)^{\ell+1}\ \frac{(1+\alpha_\ell(\omega))}{k}\ P_\ell(\cos\theta)]\ \frac{e^{ikr}}{r}$$

$$+ [\sum_{\ell=0}^{\infty} b_\ell(\omega)\ \frac{i^{\ell+1}}{k}\ P_\ell(\cos\theta)]\ \frac{e^{-ikr}}{r} \quad .$$

We can compare this asymptotic form with the one above. Since these both hold for all θ, we can equate separately coefficients of $\frac{e^{ikr}}{r}$ and $\frac{e^{-ikr}}{r}$ for each ℓ. Doing this we obtain

$$b_\ell(\omega)(-i)^{\ell+1}\ \frac{(1+\alpha_\ell(\omega))}{k} = \frac{1}{2\pi}\sqrt{\frac{mc}{\hbar}}\ k^{1/2}[\lambda_\ell(k) - \frac{1}{2k}\ (2\ell+1)],$$

$$b_\ell(\omega)\ \frac{i^{\ell+1}}{k} = \frac{1}{2\pi}\sqrt{\frac{mc}{\hbar}}\ k^{1/2}\ \frac{1}{2k}\ (-1)^\ell(2\ell+1) \quad .$$

Solving we get

$$b_\ell(\omega) = \frac{i\, k^{1/2}(2\ell+1)}{4\pi}\sqrt{\frac{m\epsilon}{\hbar}} \;.$$

$$\alpha_\ell(\omega) = \frac{2ik\lambda_\ell(k)}{2\ell+1} \;.$$

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Recalling that $f_k(\theta) = \sum_{\ell=0}^{\infty} \lambda_\ell(k)P_\ell(\cos\theta)$ we see that the second equation is a direct connection between the scattering amplitude and the function $\alpha_\ell(\omega)$ which characterizes the information about the potential which can be determined from scattering. As usual, $k = \sqrt{\frac{2m\omega}{\hbar}}$.

Although the asymptotic expressions are valid for large r we must keep in mind the restrictions $|x|,|y| << \frac{1}{2}\sqrt{\frac{\hbar}{m\omega\epsilon}}$ and $|z| << \frac{1}{\epsilon}\sqrt{\frac{\hbar}{2m\omega}}$. The dimensions of the incident wave packet are large compared to the range a of the scattering potential, but small compared to the radius r_0 associated with $\vec{r}_0$ the position of the director. Thus only the scattered outgoing component is measured by the detector.

The absolute value of the scattering amplitude can be measured experimentally by scattering probabilities, say $\frac{d\sigma}{d\Omega} = |f_k(\theta)|^2$. We ask the question: Can time delay or time of arrival measurements determine the phase of $f_k(\theta)$?

Scattering Phase Shifts

The radial function $R_{\omega\ell}(r)$ can be written in the alternate form $R_{\omega\ell}(r) = A_\ell(\omega)j_\ell(kr) + B_\ell(\omega)\eta_\ell(kr)$ for $r > a$. We define the scattering phase shift $\delta_\ell(\omega)$ to satisfy the relation $-\tan\delta_\ell(\omega) = \frac{B_\ell(\omega)}{A_\ell(\omega)}$. We can compare this with $R_{\omega\ell}(r) = (1+\alpha_\ell(\omega))h_\ell^{(1)}(kr)+h_\ell^{(2)}(kr)$, and conclude that $A_\ell(\omega) = 2+\alpha_\ell(\omega)$ and $B_\ell(\omega) = i\alpha_\ell(\omega)$. Thus

$$\tan\delta_\ell = -\frac{i\alpha_\ell(\omega)}{2+\alpha_\ell(\omega)} \text{ so that } e^{i\delta_\ell} = \cos\delta_\ell + i\sin\delta_\ell = \sqrt{1+\alpha_\ell(\omega)} .$$

Thus

$$e^{2i\delta_\ell} = 1 + \alpha_\ell(\omega) .$$

Thus we can express the scattering amplitude as

$$f_k(\theta) = \sum_{\ell=0}^{\infty} \lambda_\ell(k)P_\ell(\cos\theta) = \sum_{\ell=0}^{\infty} (2\ell+1)\,\frac{\alpha_\ell(\omega)}{2ik}\,P_\ell(\cos\theta)$$

$$= \sum_{\ell=0}^{\infty} (2\ell+1)\left[\frac{e^{2i\delta_\ell}-1}{2ik}\right]P_\ell(\cos\theta) .$$

The Time of Arrival and Time Delay Problems

Consider a scattering interaction involving a particle described by a wavefunction

$$\psi(\vec{r},t) = \int_0^\infty A(\omega)\psi_\omega(\vec{r})e^{-i\omega t}d\omega = \int_0^\infty A(\omega,\vec{r}_0)\ \psi_{\omega,\vec{r}_0}(\vec{r})e^{-i\omega t}d\omega$$

with a localized potential such that interaction with the potential is restricted to a finite interval of time, and only outgoing spherical waves arrive at the detector located at $\vec{r}_0$. The incident waves are not observed at the detector, and so the asymptotic form of $\psi_\omega(\vec{r})$ at the detector is

$$\psi_\omega(\vec r) \sim \left(\sum_{\ell=0}^{\infty} b_\ell(\omega)(-1)^{\ell+1}\frac{\alpha_\ell(\omega)}{k}P_\ell(\cos\theta)\right)\frac{e^{ikr}}{r} .$$

Substituting for $b_\ell(\omega)$ and $\alpha_\ell(\omega)$ from their derived equivalences gives

$$\psi_\omega(\vec r) \sim \frac{k^{1/2}}{2\pi}\sqrt{\frac{m\varepsilon}{\hbar}}\left(\sum_{\ell=0}^{\infty}\lambda_\ell(k)P_\ell(\cos\theta)\right)\frac{e^{ikr}}{r}$$

$$\sim \frac{k^{1/2}}{2\pi}\sqrt{\frac{m\varepsilon}{\hbar}}\, f_k(\theta)\frac{e^{ikr}}{r} .$$

Now let us phase $\psi_\omega(\vec r)$ at $\vec r_0$. From this we have

$$\psi_{\omega,\vec r_0}(\vec r) \sim \frac{k^{1/2}}{2\pi}\sqrt{\frac{m\varepsilon}{\hbar}}\, f_k'(\theta)\frac{e^{ik(r-r_0)}}{r}\frac{f_k^*(\theta_0)}{|f_k(\theta_0)|} ,$$

where $\vec r_0$ has magnitude r_0 and θ angle θ_0. Thus

$$\psi_{\omega,\vec r_0}(\vec r) = \psi_\omega(\vec r)\, e^{-ikr_0}\frac{f_k^*(\theta_0)}{|f_k(\theta_0)|}$$

and consequently

$$A(\omega,\vec r_0) = A(\omega)\, e^{ikr_0}\frac{f_k(\theta_0)}{|f_k(\theta_0)|} .$$

Now let us take a narrow wave packet in frequency space $A(\omega)$ distributed about some ω_0, and determine the time of arrival at $\vec r_0$ and some time delay values. Let

$$e^{i\eta_k(\theta)} = \frac{f_k(\theta)}{|f_k(\theta)|}$$

define the phase $\eta_k(\theta)$ of the scattering amplitude $f_k(\theta)$. Then

$$A(\omega,\vec{r}_0) = A(\omega)e^{i(kr_0+\eta_k(\theta))} .$$

Let us choose a particular form for $A(\omega)$ which is narrow about ω_o and square normalized. We take the dummy expression $A(\omega) = \sqrt{\delta(\omega-\omega_o)}$, $\omega_o > 0$. In practice, we have to take non-zero square normalized functions with a parameter that is non-zero, but selected to approach $\sqrt{\delta(\omega-\omega_o)}$ as the parameter approaches zero. We then perform the required integrations for non-zero values of the parameter, and take the limit to zero after. In practice we can avoid these steps by the following formal operations.

$$\langle t\rangle_{\vec{r}_0} = \int_o^\infty A^*(\omega,\vec{r}_0)[-i\,\frac{\partial}{\partial\omega}]A(\omega,\vec{r}_0)d\omega ,$$

$$= \int_o^\infty A^*(\omega)e^{-i(kr_0+\eta_k(\theta))}[-i\,\frac{\partial}{\partial\omega}]\{A(\omega)e^{i(kr_0+\eta_k(\theta))}\}d\omega ,$$

$$= \int_o^\infty A^*(\frac{\hbar k^2}{2m})e^{-i(kr_0+\eta_k(\theta))}[-i\,\frac{\partial}{\partial k}]\{A(\frac{\hbar k^2}{2m})e^{i(kr_0+\eta_k(\theta))}\}dk .$$

We now use the relation $A(\omega) = \sqrt{\delta(\omega-\omega_o)}$ to get

$$A(\frac{\hbar k^2}{2m}) = \sqrt{\delta(\frac{\hbar}{2m}[k^2-k_0^2])} = \sqrt{\frac{m}{\hbar k_0}}\,\sqrt{\delta(k-k_0)} .$$

Thus

$$\langle t\rangle_{\vec{r}_0} = \frac{m}{\hbar k_0}\int_o^\infty \sqrt{\delta(k-k_0)}\,e^{-i(kr_0+\eta_k(\theta))}[-i\,\frac{\partial}{\partial k}]\{\sqrt{\delta(k-k_0)}\,e^{i(kr_0+\eta_k(\theta))}\}dk$$

$$= \frac{m}{\hbar k_0}\,[r_0 + \frac{\partial}{\partial k_0}\,\eta_{k_0}(\theta)] .$$

To obtain the time delay corresponding to ∂t in the classical case we ask what is the expected time of arrival of a free particle wave packet with the same form as the given wave packet before scattering at a point of distance r_0 from the origin along the z axis after passing through the origin. Before scattering, only the plane wave component contributes and so

$$\psi_\omega(\vec{r}) = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{m\epsilon}{\hbar}}\, k^{1/2}\, e^{ikz} \quad \text{and} \quad A(\omega) = \sqrt{\frac{m}{\hbar k_0}}\, \sqrt{\delta(k-k_0)} \ .$$

The expression for $\psi_\omega(\vec{r})$ is valid for $|x|, |y| << \frac{1}{2}\sqrt{\frac{\hbar}{m\omega\epsilon}}$ and $|z| << \frac{1}{\epsilon}\sqrt{\frac{\hbar}{2m\omega}}$. Assume that $z = r_0$ is within this range (although x and $y \tilde{=} r_0$ will not be in general). If we define $\vec{r}_0$ for this case by $z = r_0$ and $x = y = 0$ as the components for $\vec{r}_0$, and measure expected time of arrival we get (for the free particle)

$$\langle t\rangle^{f}_{\vec{r}_0} = \int_0^\infty A^*(\omega,\vec{r}_0)\left[-i\frac{\partial}{\partial\omega}\right]A(\omega,\vec{r}_0)d\omega \ ,$$

where

$$\psi_{\omega,\vec{r}_0}(\vec{r}) = \frac{1}{\sqrt{2\pi}}\sqrt{\frac{m\epsilon}{\hbar}}\, k^{1/2}\, e^{ik(z-r_0)}$$

and so

$$A(\omega,\vec{r}_0) = A(\omega)\, e^{ikr_0} = \sqrt{\frac{m}{\hbar k_0}}\,\sqrt{\delta(k-k_0)}\, e^{ikr_0} \ .$$

Thus

$$\langle t\rangle^{f}_{\vec{r}_0} = \frac{m}{\hbar k_0}\int_0^\infty \sqrt{\delta(k-k_0)}\, e^{-ikr_0}\left[-i\frac{\partial}{\partial k}\right]\left\{\sqrt{\delta(k-k_0)}\, e^{ikr_0}\right\}dk$$

$$= \frac{mr_0}{\hbar k_0} \ .$$

Thus we compute the time delay ∂t a function of k_0 and θ as

$$\partial t = \langle t\rangle_{\vec{r}_0} - \langle t\rangle^{f}_{\vec{r}_0}$$

$$= \frac{m}{\hbar k_0}\frac{\partial}{\partial k_0}\eta_{k_0}(\theta) \ .$$

Observe that ∂t is independent of r_0.

In essence, we can determine the phase $\eta_k(\theta)$ of the scattering amplitude from the time delay $\partial t(k,\theta)$. We have

$$\partial t(k,\theta) = \frac{m}{\hbar k}\frac{\partial}{\partial k}\eta_k(\theta) \quad \text{and so} \quad \eta_k(\theta) = \frac{\hbar}{m}\int^k \partial t(k,\theta)k\,dk \ .$$

It appears that $\eta_k(\theta)$ is not completely determined by this integral, but rather we can add an arbitrary function of θ, independent of k to $\eta_k(\theta)$ and still have the same time delay ∂t. This arbitrary function can be determined by examining the behavior of the phase $\eta_k(\theta)$ of the scattering amplitude $f_k(\theta)$ for $k \to 0^+$ or $k \to +\infty$. Under these circumstances we can obtain $\eta_k(\theta)$ and $\frac{d\sigma}{d\Omega} = |f_k(\theta)|^2$ from experimental measurements, and consequently we know $f_k(\theta)$. It remains to relate $f_k(\theta)$ to the potential $V(r)$ and consider the phase of $f_k(\theta)$ for limiting values of k.

Green's Function Solution to the Radial Schrödinger Equation

Consider the equation

$$-\frac{\hbar^2}{2m}U''(r) + [\frac{\hbar^2 \ell(\ell+1)}{2mr^2} + V(r)]U(r) = \hbar\omega U(r).$$

It can be rewritten as

$$U''(r)+k^2U(r) = [\frac{\ell(\ell+1)}{r^2} + \frac{2m}{\hbar^2}V(r)]U(r) \text{ , } k^2 = \frac{2m\omega}{\hbar} \text{ ,}$$

or $U''(r) + (k^2 - \frac{\ell(\ell+1)}{r^2})U(r) = \frac{2m}{\hbar^2}V(r)U(r)$. The inhomogeneous equation $U''(r) + (k^2 - \frac{\ell(\ell+1)}{r^2})U(r) = F(r)$ has the Green's function solution $U(r) = \int_0^\infty G(r,s)F(s)ds$ where $G(r,s)$ satisfies $\frac{\partial^2}{\partial s^2}G(r,s) + (k^2 - \frac{\ell(\ell+1)}{s^2})G(r,s) = \delta(r-s)$ plus boundary conditions. Thus

$$G(r,s) = A(r)sh_\ell^{(1)}(ks) + B(r)sh_\ell^{(2)}(ks) \qquad \text{for} \quad 0 < r < s \text{ ,}$$

$$= C(r)sj_\ell(ks) + D(r)sn_\ell(ks) \qquad \text{for} \quad r > s > 0 \text{ .}$$

$G(r,0) = 0 \rightarrow D(r) = 0$. We choose a Green's function for outgoing spherical waves as $s \rightarrow +\infty$. Hence $B(r) = 0$. Thus

$$G(r,s) = A(r)sh_\ell^{(1)}(ks) \qquad \text{for} \quad r < s \text{ ,}$$

$$= C(r)sj_\ell(ks) \qquad \text{for} \quad r > s \text{ .}$$

To determine $A(r)$ and $C(r)$ we have two more equations, namely

$$G(r,r^{+}) = G(r,r^{-}) \qquad \text{and} \qquad \frac{d}{ds}\, G(r,s)\Big|_{r^{-}}^{r^{+}} = 1 \; .$$

From these equations we get

$$A(r) = \frac{j_\ell(kr)}{kr[j_\ell(kr)h_\ell^{(1)\prime}(kr) - h_\ell^{(1)}(kr)j_\ell'(kr)]} \; ,$$

$$C(r) = \frac{h_\ell^{(1)}(kr)}{kr[j_\ell(kr)h_\ell^{(1)\prime}(kr) - h_\ell^{(1)}(kr)j_\ell'(kr)]} \; .$$

The factor in the denominator, $r(j_\ell(kr)kh_\ell^{(1)\prime}(kr)-h_\ell^{(1)}(kr)kj_\ell'(kr))$ is equal to $\frac{i}{kr}$ and so $A(r) = -kirj_\ell(kr)$ and $C(r) = -kirh_\ell^{(1)}(kr)$. Therefore,

$$G_\ell(r,s) = -irskj_\ell(kr)h_\ell^{(1)}(ks) \qquad \text{for} \qquad r < s \; ,$$

$$G_\ell(r,s) = -irskh_\ell^{(1)}(kr)j_\ell(ks) \qquad \text{for} \qquad r > s \; .$$

Since the radial wave function is (for $r > a$),

$$R_{\omega\ell}(r) = (1+\alpha_\ell(\omega)\,)h_\ell^{(1)}(kr)+h_\ell^{(2)}(kr) \; ,$$

we get

$$U_{\omega\ell}(r) = (1+\alpha_\ell(\omega))rh_\ell^{(1)}(kr)+rh_\ell^{(2)}(kr) \; .$$

The portion contributed by the incident wave is

$$rh_\ell^{(1)}(kr)+rh_\ell^{(2)}(kr) = 2rj_\ell(kr) \; .$$

The Green's function solution is

$$U_{\omega,\ell}(r) = 2rj_\ell(kr) + \frac{2m}{\hbar^2}\int_0^\infty G_\ell(r,s)V(s)U_{\omega\ell}(s)ds \quad .$$

This is the integral equation for the radial solution $U_{\omega,\ell}(r)$. Furthermore $U_{\omega,\ell}(r) = 2rj_\ell(kr)+a_\ell(\omega)rh_\ell^{(1)}(kr)$ for $r > a$, and so for $r > a$,

$$a_\ell(\omega)rh^{(1)}(kr) = \frac{2m}{\hbar^2}\int_0^a G_\ell(r,s)V(s)U_{\omega\ell}(s)ds \quad .$$

$r > s$ in this integral, and so $G_\ell(r,s) = -irskh_\ell^{(1)}(kr)j_\ell(ks)$. Consequently we get

$$a_\ell(\omega) = -\frac{2mik}{\hbar^2}\int_0^a sj_\ell(ks)V(s)U_{\omega\ell}(s)ds \quad .$$

The upper limit a can of course be extended to infinity. We assumed $V(s) = 0$ for $s > a$ for simplicity.

The Born Approximation

The approximate substitution $U_{\omega\ell}(s) = 2sj_\ell(ks)$ into

$$a_\ell(\omega) = -\frac{2mik}{\hbar^2}\int_0^\infty sj_\ell(ks)V(s)U_{\omega\ell}(s)ds$$

is called the Born Approximation. It is valid in general for weak finite potentials and high initial energies. In this approximation,

$$a_\ell(\omega) = -\frac{4mik}{\hbar^2}\int_0^\infty s^2[j_\ell(ks)]^2V(s)ds \quad .$$

Observe that $\alpha_\ell(\omega)$ is imaginary negative for a positive potential $V(s)$. Since $\alpha_\ell(\omega) = \frac{2ik\lambda_\ell(k)}{2\ell+1}$, $\lambda_\ell(k)$ is negative real, and since $f_k(\theta) = \sum_{\ell=0}^{\infty} \lambda_\ell(k)P_\ell(\cos\theta)$, $f_k(\theta)$ is real in this approximation. For $f_k(\theta)$ non-zero we see that there is no time delay in the Born Approximation. The values of θ which make $f_k(\theta) = 0$ for fixed k are the angles identifying regions of destructive interference in the pattern of interference fringes for $\frac{d\sigma}{d\Omega} = |f_k(\theta)|^2$. For any θ and k for which $f_k(\theta) \neq 0$ there is a non-zero probability of arrival, and time delay ∂t can be measured and will always turn out to be zero. If $f_k(\theta) = 0$, the probability of arrival is zero and the time delay concept at this point for this energy is nonsense. This reflects our inability to determine the phase of $f_k(\theta)$ at this point.

Although $\partial t = 0$ in the Born approximation, this is not true of higher approximations or the exact solution in general.

S-Wave ($\ell = 0$) Scattering in the Born Approximation

First we observe that $j_0(ks) = \frac{\sin ks}{ks}$ and so

$$\alpha_0(\omega) = -\frac{4mi}{\hbar^2 k}\int_0^\infty \sin^2 ks V(s)ds \quad ,$$

and hence

$$\alpha_0(\omega) + \frac{2mi}{\hbar^2 k}\int_0^\infty V(s)ds = \frac{2mi}{\hbar^2 k}\int_0^\infty \cos(2ks)V(s)ds \quad .$$

The trick for inversion here is as follows. $V(s)$ is defined only for $s > 0$. Extend the definition of $V(s)$ for $s < 0$ by $V(-s) = V(s)$ (even function). Then

$$\alpha_0\left(\frac{\hbar k^2}{2m}\right) + \frac{mi}{\hbar^2 k}\int_{-\infty}^{\infty} V(s)ds = \frac{mi}{\hbar^2 k}\int_{-\infty}^{\infty}\cos(2ks)V(s)ds$$

$$= \frac{mi}{\hbar^2 k}\int_{-\infty}^{\infty} e^{2iks}V(s)ds \quad .$$

Hence

$$\frac{\hbar^2 k}{mi}\alpha_0\left(\frac{\hbar k^2}{2m}\right) + \int_{-\infty}^{\infty} V(s)ds = \int_{-\infty}^{\infty} e^{2iks}V(s)ds \quad .$$

Multiply by $\frac{1}{2\pi}e^{-2iks'}$ and integrate over k from $-\infty$ to ∞ and simplify to get

$$V(r) = \frac{2}{\pi}\frac{h^2}{mi}\int_0^{\infty} k\alpha_0\left(\frac{\hbar k^2}{2m}\right)\cos(2kr)dk \ , \quad \text{for} \quad r > 0 \ ,$$

$$= \frac{2h}{i\pi}\int_0^{\infty}\alpha_0(\omega)\cos\left(2\sqrt{\frac{2m\omega}{h}}\ r\right)d\omega \ .$$

Using $\alpha_0(\omega) = 2ik\lambda_0(k)$ and $\lambda_0(k) = \frac{1}{2}\int_0^{\pi} f_k(\theta)\sin\theta d\theta$ we get

$$V(r) = \frac{2}{\pi}\frac{h^2}{m}\int_0^{\infty} k^2\left[\int_0^{\pi} f_k(\theta)\sin\theta d\theta\right]\cos(2kr)dk \ , \quad r > 0$$

in the Born approximation for the real scattering amplitude $f_k(\theta)$.

Low Energy Scattering

Suppose the potential $V(r)$ has range a and $ka \ll 1$. Let us solve the radial Schrödinger equation by Green's functions in this low energy limit. We have the equations

$$U_{\omega,\ell}(r) = 2rj_\ell(kr) + \frac{2m}{\hbar^2}\int_0^a G_\ell(r,s)V(s)U_{\omega,\ell}(s)ds$$

for $r < a$, and for $r > s$,

$$G_\ell(r,s) = -irskh_\ell^{(1)}(kr)j_\ell(ks)$$

and

$$\alpha_\ell(\omega) = -\frac{2mik}{\hbar^2}\int_0^a sj_\ell(ks)V(s)U_{\omega,\ell}(s)ds \quad .$$

Since $ka \ll 1$, we can use the asymptotic forms

$$j_\ell(kr) \sim \frac{2^\ell \ell!}{(2\ell+1)!}(kr)^\ell \qquad \text{and} \qquad h_\ell^{(1)}(kr) \sim \frac{(2\ell)!}{i2^\ell \ell!}(kr)^{-\ell-1} \quad .$$

In this limiting approximation, $G_\ell(r,s) = -\frac{r^{-\ell}s^{\ell+1}}{2\ell+1}$ for $r > s$ and $G_\ell(r,s) = -\frac{s^{-\ell}r^{\ell+1}}{2\ell+1}$ for $r < s$.

The W.K.B. Approximation for the Radial Schrödinger Equation

Let us look for a semi-classical approximation relating the potential $V(r)$ to the functions $\alpha_\ell(\omega)$. The Schrödinger equation is

$$U''(r) + (k^2 - \frac{\ell(\ell+1)}{r^2})U(r) = \frac{2m}{\hbar^2}V(r)U(r)$$

with a solution $U_{\omega\ell}(r)$ satisfying $U_{\omega\ell}(r) = 2rj_\ell(kr)+\alpha_\ell(\omega)rh_\ell^{(1)}(kr)$ for $r > a$. We assume the potential $V(r)$ has the following very special properties:

(1) $V(r)$ is bounded, $V(r) \leq V(0)$ for all $r \geq 0$, $V(0)$ finite.

(2) $V(r)$ defined on $0 < r < a$ is strictly monotone decreasing in r.

(3) $V(r) = 0$ for $r \geq a$, $V(r) > 0$ for $r < a$.

This form is sufficiently general for present purposes. Under some conditions, one or more of the above restrictions may be relaxed.

The approximation we will consider is one of large k (high energy); we suppose $\frac{\hbar^2 k^2}{2m} \gg V(0)$ and that V is slowly varying over the range of one wavelength. As a boundary condition we will insist that $U_{\omega\ell}(0) = 0$.

S Wave ($\ell = 0$) Solution

This is the only case via which the W.K.B. approximation will work. $U_{\omega 0}(r)$ satisfies the equation

$$U''(r) + k^2 U(r) = \frac{2m}{\hbar^2} V(r) U(r) \quad \text{for} \quad r > 0 \text{ , and}$$

$$U_{\omega,0}(r) = \frac{2 \sin kr}{k} - i\alpha_0(\omega) \frac{e^{ikr}}{k} \quad \text{for} \quad r > a \text{ ;} \quad U_{\omega 0}(0) = 0 \text{ .}$$

We apply the W.K.B. approximation on the interval $0 < r < a$. $U(r)$ satisfies the ordinary one-dimensional Schrödinger equation here, and so

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the solution is of the form (boundary condition at $r = 0$ imposed)

$$U_{\omega,0}(r) \cong \frac{A}{[k^2 - \frac{2m}{\hbar^2} V(r)]^{1/4}} \sin\left(\int_0^r [k^2 - \frac{2mV(s)}{\hbar^2}]^{1/2} ds\right) .$$

This approximate solution is valid for all $r > 0$. In particular we insist that this solution be exact for $r > a$. In this case;

$$U_{\omega,0}(r) \underset{(r>a)}{=} Ak^{-(1/2)} \sin\left(\int_0^a [k^2 - \frac{2mV(s)}{\hbar^2}]^{1/2} ds + k(r-a)\right) .$$

For simplicity let $\gamma(k) = \int_0^a [k^2 - \frac{2mV(s)}{\hbar^2}]^{1/2} ds - ka$. Then

$$U_{\omega,0}(r) = Ak^{-(1/2)} \sin(\gamma(k)+kr) \qquad \text{for } r > a ,$$

$$= \frac{2 \sin kr}{k} - i\alpha_0(\omega) \frac{e^{ikr}}{k} \qquad \text{for } r > a .$$

Comparison gives the solutions

$$Ak^{-(1/2)} \cos \gamma(k) = \frac{2}{k} + \frac{\alpha_0(\omega)}{k} ,$$

$$Ak^{-(1/2)} \sin \gamma(k) = - \frac{i}{k} \alpha_0(\omega) .$$

Divide to get $\tan \gamma(k) = - \frac{i\alpha_0(\omega)}{2+\alpha_0(\omega)} = \tan \delta_0(k)$. We have $\gamma(k) = \delta_0(k)$ the s - wave scattering phase shift. Thus

$$\delta_0(k) = \int_0^a [k^2 - \frac{2m}{\hbar^2} V(s)]^{1/2} ds - ka .$$

Define k' in terms of s by $k' = \sqrt{\frac{2m}{\hbar^2} V(s)}$ a monotone decreasing positive function of s for $0 < s < a$. Then $s = V^{-1}(\frac{\hbar^2 k'^2}{2m})$. We have

$$\delta_0(k) = - \int_o^{k'_0} [k^2 - k'^2]^{1/2} V^{-1\prime}(\frac{\hbar^2 k'^2}{2m}) \frac{\hbar^2}{m} k' dk' - ka \quad ,$$

so

$$\delta'_0(k) = \frac{d}{dk} \delta_0(k) = - \frac{\hbar^2 k}{m} \int_o^{k'_0} \frac{V^{-1\prime}(\frac{\hbar^2 k'^2}{2m}) k' dk'}{\sqrt{k^2 - k'^2}} - a \quad .$$

(Here $k'_0 = \sqrt{\frac{2m\ V(0)}{\hbar^2}}$) . Transforming the integration from k' to $\omega' = \frac{\hbar k'^2}{2m}$ we get

$$\delta'_0(k) = \delta'_0(\sqrt{\frac{2m\omega}{\hbar}}) = - \hbar \omega^{1/2} \int_o^{\omega'_0} \frac{V^{-1\prime}(\hbar\omega') d\omega'}{\sqrt{\omega - \omega'}} - a$$

where $\omega = \frac{\hbar k^2}{2m}$ and $\omega'_0 = \frac{\hbar k'^2_0}{2m}$. We now make the approximation $\omega'_0 = \omega$. This means the potential $V(r)$ rises to $+\infty$ very rapidly as r decreases to zero, and the equation can be placed in the invertible form

$$g(\omega) = \int_o^{\omega} \frac{h(\omega') d\omega'}{\sqrt{\omega - \omega'}} \qquad \text{with} \qquad g(\omega) = \frac{\delta'_0(\sqrt{\frac{2m\omega}{\hbar}}) + a}{\omega^{1/2}}$$

and $h(\omega') = -\hbar V^{-1\prime}(\hbar\omega')$ where the inversion integral is

$$h(\omega') = \frac{1}{\pi} \frac{\partial}{\partial \omega'} [\int_o^{\omega'} \frac{g(\omega) d\omega}{\sqrt{\omega' - \omega}}] \quad .$$

Substituting into the inversion integral and integrating with respect to ω we obtain

$$V^{-1}(\hbar\omega') = \frac{1}{\pi}\int_0^{\omega'} \frac{\delta_0'(\sqrt{\frac{2m\omega}{\hbar}})\omega^{-(1/2)}d\omega}{\sqrt{\omega'-\omega}}$$

where $\delta_0'(k) = \frac{d}{dk}\delta_0(k)$ and the constant of integration has been taken as zero. (As $\omega' \to \infty$ both sides assumed to approach zero.) Changing the variable of integration to k we have

$$V^{-1}\left(\frac{\hbar^2k'^2}{2m}\right) = \frac{2}{\pi}\int_0^{k'} \frac{\delta_0'(k)dk}{\sqrt{k'^2-k^2}} \quad .$$

We can compare the above equation with the classical time delay on reflection equation namely

$$V^{-1}\left(\frac{mu}{2}\right) = -\frac{1}{\pi}\int_0^{u^{1/2}} \frac{\partial t(0,v_0)v_0dv_0}{\sqrt{u-v_0^2}}$$

and using $u = \frac{\hbar^2k'^2}{m^2}$ and $v_0 = \frac{\hbar k}{m}$ we see $\delta_0'(k) = -\frac{1}{2}\frac{\hbar k}{m}\partial t(0, \frac{\hbar k}{m})$ the first direct connection between classical time delay and approximate scattering phase shifts. Note that a zero phase shift $\delta_0(k) = 0$ means $V^{-1}(\frac{\hbar^2k'^2}{2m}) = 0$ and so $V(r) \sim \alpha\delta(r)$ which is the zero potential with an infinite peak at $r = 0$.

The Second Born Approximation

We recall that in the Born Approximation, $\alpha_\ell(\omega)$ was given by $\alpha_\ell(\omega) = -\frac{4mik}{\hbar^2}\int_0^\infty s^2[j_\ell(ks)]^2V(s)ds$. This gave us the approximate

$U_{\omega\ell}(r)$ for $r > a$ namely $U_{\omega\ell}(r) = 2rj\,(kr)+\alpha_\ell(\omega)rh_\ell^{(1)}(kr)$. From the integral equation

$$U_{\omega\ell}(r) = 2rj_\ell(kr) + \frac{2m}{\hbar^2}\int_0^a G_\ell(r,s)V(s)U_{\omega\ell}(s)ds$$

we can get an approximate behavior for $U_{\omega\ell}(r)$ when $r < a$ by substituting the crude approximation $U_{\omega\ell}(s) = 2sj_\ell(ks)$ for $s < a$ into this integral. For $r < a$ we split the integral up so that

$$\begin{aligned}
U_{\omega\ell}(r) &= 2rj_\ell(kr) + \frac{2m}{\hbar^2}\int_0^r G_\ell(r,s)V(s)U_{\omega\ell}(s)ds \\
&\quad + \frac{2m}{\hbar^2}\int_r^a G_\ell(r,s)V(s)U_{\omega\ell}(s)ds \\
&= 2rj_\ell(kr) - \frac{2mkirh_\ell^{(1)}(kr)}{\hbar^2}\int_0^r Sj_\ell(ks)V(s)U_{\omega\ell}(s)ds \\
&\quad - \frac{2mkirj_\ell(kr)}{\hbar^2}\int_r^a sh_\ell^{(1)}(ks)V(s)U_{\omega\ell}(s)ds \quad \text{for } r < a\,.
\end{aligned}$$

For the Born approximation we substitute $U_{\omega\ell}(s) = 2sj_\ell(ks)$ into this integral and get

$$\begin{aligned}
U_{\omega\ell}(r) \doteq 2rj_\ell(kr) &- \frac{4mkirh_\ell^{(1)}(kr)}{\hbar^2}\int_0^r s^2[j_\ell(ks)]^2V(s)ds \\
&- \frac{4mkirj_\ell(kr)}{\hbar^2}\int_r^a s^2h_\ell^{(1)}(ks)j_\ell(ks)V(s)ds \quad ,
\end{aligned}$$

for $r < a$, the range of the potential. $\alpha_\ell(\omega)$ in the second Born approximation is found by substituting $U_{\omega\ell}(r)$ as given above into

$$\alpha_\ell(\omega) = -\frac{2mik}{\hbar^2}\int_0^a r j_\ell(kr)V(r)U_{\omega\ell}(r)dr$$

to get

$$\alpha_\ell(\omega) \doteq -\frac{4mik}{\hbar^2}\int_0^a r^2[j_\ell(kr)]^2V(r)dr$$

$$-\frac{8m^2k^2}{\hbar^4}\int_0^a dr\ r^2 j_\ell(kr)h_\ell^{(1)}(kr)V(r)[\int_0^r s^2[j_\ell(ks)]^2V(s)ds]$$

$$-\frac{8m^2k^2}{\hbar^4}\int_0^a dr\ r^2[j_\ell(kr)]^2V(r)[\int_r^a s^2h_\ell^{(1)}(ks)j_\ell(ks)V(s)ds] \quad .$$

If we write the latter integral in the plane and interchange the order of integration, we see it is the same as the preceding one and so $\alpha_\ell(\omega)$ can be given (in the second Born approximation) by

$$\alpha_\ell(\omega) = -\frac{4mik}{\hbar^2}\int_0^a r^2[j_\ell(kr)]^2V(r)dr$$

$$-\frac{16m^2k^2}{\hbar^4}\int_0^a dr\ r^2 j_\ell(kr)h_\ell^{(1)}(kr)V(r)[\int_0^r s^2[j_\ell(ks)]^2V(s)ds] \quad .$$

We assume that the Born approximation holds, and so the first t erm above, although small, is much larger than the second term. Observe that $h_\ell^{(1)}(kr) = j_\ell(kr) + i\eta_\ell(kr)$. We are interested in obtaining the approximate value of the small imaginary part of $\alpha_\ell(\omega)$ and the much smaller real part of $\alpha_\ell(\omega)$. Since the first Born approximation gives us a reasonable value for the imagingary part of $\alpha_\ell(\omega)$, we ignore the imaginary contribution of $i\eta_\ell(kr)$ and simply replace $h_\ell^{(1)}(kr)$ by $j_\ell(kr)$.

This means we can explicitly integrate the second order term and we have the approxiamtion,

$$\alpha_\ell(\omega) = -\frac{4mik}{\hbar^2}\int_0^a r^2[j_\ell(kr)]^2 V(r)dr - \frac{8m^2k^2}{\hbar^4}\left[\int_0^a s^2[j_\ell(ks)]^2 V(s)ds\right]^2$$

The condition for validity of the Born approximation is $\frac{2mk}{\hbar^2}\int_0^a r^2[j_\ell(kr)]^2 V(r)dr << 1$. Observe that the error or uncertainly in this first term is small compared to the first term but of the same order as the much smaller second term. Also observe that we can reformulate the condition of validity of the approximation for large k by using the asymptotic form (for large arguments) of $j_\ell(kr)$. The condition looks like $\int_0^a V(r)dr << \hbar v$ where v is $\frac{\hbar k}{m}$ the velocity. (For large k and slowly varying V we replace $(kr)^2[j_\ell(kr)]^2$ by $\frac{1}{2}$ in the integral). This inequality does not hold in classical physics for large k and small $\hbar$.

The W.K.B. Approximation in General

The failure of the Born Approximation to apply in the classical limit forces use to return to the W.K.B. approximation. Recall that we had

$$\delta_0(k) = -\int_0^{k_0'} [k^2-k'^2]^{1/2} V^{-1'}\left(\frac{\hbar^2k'^2}{2m}\right)\frac{\hbar^2}{m}\,k'dk' - ka$$

where $k_0' = \sqrt{\frac{2mV(0)}{\hbar}}$ was taken as k in the case that $V(0)$ was infinite. For $V^{-1'}$, the ' of course means differentiation with respect to the argument of V^{-1} which has units of energy. We can change the variable of integration to ω to get

$$\delta_0\left(\sqrt{\frac{2m\omega}{\hbar}}\right) = -\sqrt{2m\hbar}\int_0^{\omega}(\omega-\omega')^{1/2}V^{-1'}(\hbar\omega')d\omega' - ka$$

$$= \lim_{a\to\infty}\left[-\sqrt{2m\hbar}\int_{\frac{v(a)}{\hbar}}^{\omega}(\omega-\omega')^{1/2}V^{-1'}(\hbar\omega')d\omega' - ka\right] .$$

Recall that $V^{-1'} = \frac{d}{d(\hbar\omega)}V^{-1}$. If $V^{-1'}$ is very large (and negative) for ω' near zero, but contributes little for larger ω' we can approximate $(\omega-\omega')^{1/2}$ by $\omega^{1/2}$ and in this case we have explicitly $\delta_0\left(\sqrt{\frac{2m\omega}{\hbar}}\right) \sim -kV^{-1}(\hbar\omega)$ as a crude estimate.

Alternatively, we could try integration by parts in the expression

$$\delta_0\left(\sqrt{\frac{2m\omega}{\hbar}}\right) = \lim_{a\to\infty}\left[-\sqrt{2m\hbar}\int_{\frac{v(a)}{\hbar}}^{\omega}(\omega-\omega')^{1/2}V^{-1'}(\hbar\omega')d\omega' - ka\right] .$$

Doing this we get

$$\delta_0\left(\sqrt{\frac{2m\omega}{\hbar}}\right) = \lim_{a\to\infty}\left[-\sqrt{2m\hbar}\left\{-\omega^{1/2}\frac{a}{\hbar} + \frac{1}{2\hbar}\int_{\frac{v(a)}{\hbar}}^{\omega}\frac{V^{-1}(\hbar\omega')d\omega'}{(\omega-\omega')^{1/2}}\right\} - ka\right]$$

$$= -\sqrt{\frac{m}{2\hbar}}\int_0^{\omega}\frac{V^{-1}(\hbar\omega')d\omega'}{(\omega-\omega')^{1/2}} .$$

This gives the much better estimate

$$\delta_0\left(\sqrt{\frac{2m\omega}{\hbar}}\right) = -\sqrt{\frac{m}{2\hbar}}\int_0^{\omega}\frac{V^{-1}(\hbar\omega')d\omega'}{(\omega-\omega')^{1/2}} .$$

This expression can be inverted as before, and the result is

$$V^{-1}(\hbar\omega') = -\sqrt{\frac{2\hbar}{m}}\ \frac{1}{\pi}\ \frac{\partial}{\partial\omega'}\ [\int_0^{\omega'} \frac{\delta_0(\sqrt{\frac{2m\omega}{\hbar}})d\omega}{\sqrt{\omega'-\omega}}]\ .$$

W.K.B. Approximation for Larger $\ell > 0$

For $\ell > 0$, the Schrödinger equation for $U_{\omega\ell}(r)$ becomes

$$-\frac{\hbar^2}{2m} U''(r) + (V(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2})U(r) = \hbar\omega U(r)\quad .$$

The potential function in this case is $V(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}$, $r > 0$. For each energy level $\hbar\omega$ there is a classical turning point $R_\ell(\omega)$ such that $R_\ell(\omega) = V_\ell^{-1}(\hbar\omega)$ where V_ℓ is the modified potential $V_\ell(r) = V(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}$. For $r > R_\ell(\omega)$ the solution $U(r)$ is oscillatory, and for $r < R_\ell(\omega)$, $U(r)$ degenerates to zero as $r \to 0$. Let us assume we have a real function $U(r)$ satisfying the differential equation above and the boundary condition at 0. We will ignore the normalization factor on $U(r)$. The standard W.K.B. approximation across Classical turning points (with the connection formula) gives us the form

$$U(r) = \frac{2}{\sqrt[4]{k^2 - \frac{2m\ V_\ell(r)}{\hbar^2}}} \cos\ (\int_{R_\ell(\omega)}^{r} \sqrt{k^2 - \frac{2mV_\ell(s)}{\hbar^2}}\ ds - \frac{\pi}{4})$$

for $r > R_\ell(\omega)$. (See Merzbacher page 121, equation 7.26(a).)

Let us now look at the asymptotic behavior of this expression for large r. For a real solution to the radial equation of the form

$U(r) = A_\ell(k) r j_\ell(kr) + B_\ell(k) r \eta_\ell(kr)$ for $r > 0$ we observe that $-\tan\delta_\ell = \dfrac{B_\ell(k)}{A_\ell(k)}$ defines the scattering phase shift $\delta_\ell(k)$ and moreover the asymptotic form of $U(r)$ for large r involves the phase shift as

$$U(r) \sim C_\ell(k) \sin(kr - \ell\pi/2 + \delta_\ell(k)) \quad .$$

A comparison tells us that since $\cos x = \sin(\frac{\pi}{2} + x)$, we have

$$\delta_\ell(k) = (2\ell+1)\frac{\pi}{4} - kr + \int_{V_\ell^{-1}(\hbar\omega)}^{r} \sqrt{k^2 - \frac{2mV_\ell(s)}{\hbar^2}}\, ds \quad \text{as} \quad r \to +\infty \; .$$

This is valid for $\ell \geq 1$ and not for $\ell = 0$. For $\ell = 0$ we cannot state that negative exponent only contributes for $r < R_\ell(\omega) = R_0(\omega)$. This case $\ell = 0$ has been dealt with above. (See Merzbacher page 121 equations (7.26a) and (7.26b) and examine the behavior of the wavefunction in the $0 < r < R_\ell(\omega)$ region. Remember $U(r) \to 0$ as $r \to 0$.)

Phase Error in Approximation

Because the W.K.B. approximation method is not exact, we can expect that the phase term $(2\ell+1)\frac{\pi}{4}$ above will be close but not exactly correct, as a result of phasing for large r. To recalculate this phase we set $V(s) = 0$ so $V_\ell(s) = \dfrac{\hbar^2 \ell(\ell+1)}{2ms^2}$. Also $V_\ell^{-1}(\hbar\omega) = \dfrac{\sqrt{\ell(\ell+1)}}{k}$. We calculate $\displaystyle\int_{\frac{\sqrt{\ell(\ell+1)}}{k}}^{r} \sqrt{k^2 - \frac{\ell(\ell+1)}{s^2}}\, ds$ for large r and find that it approaches

$kr - \sqrt{\ell(\ell+1)}\,\frac{\pi}{2}$. We know $\delta_\ell(k) = 0$ for $V(r) = 0$ and consequently $(2\ell+1)\,\frac{\pi}{4}$ should be replaced by $\sqrt{\ell(\ell+1)}\,\frac{\pi}{2}$. This gives us the relation

$$\delta_\ell(k) = \sqrt{\ell(\ell+1)}\,\frac{\pi}{2} + \lim_{r \to \infty} \left[-kr + \int_{V^{-1}\left(\frac{\hbar^2 k^2}{2m}\right)}^{r} \sqrt{k^2 - \frac{2mV_\ell(s)}{\hbar^2}}\; ds\right]$$

$$= \sqrt{\ell(\ell+1)}\,\frac{\pi}{2} + \lim_{r \to \infty} \left[-kr + \int_{k}^{\sqrt{\frac{2mV_\ell(r)}{\hbar^2}}} \sqrt{k^2 - k'^2}\; V_\ell^{-1'}\left(\frac{\hbar^2 k'^2}{2m}\right) \frac{\hbar^2}{m}\, k'dk'\right] .$$

As $r \to \infty$, $V(r) \to 0$ and so for $r > a$, $V_\ell(r) = \frac{\hbar^2 \ell(\ell+1)}{2mr^2}$ and the upper limit of integration is $\sqrt{\frac{\ell(\ell+1)}{r}}$. We can switch variables form k' to ω' in the integration, using $k = \sqrt{\frac{2m\omega}{\hbar}}$ and $k' = \sqrt{\frac{2m\omega'}{\hbar}}$ to get

$$\delta_\ell(k) = \sqrt{\ell(\ell+1)}\,\frac{\pi}{2} + \lim_{r \to \infty} \left[-kr - \sqrt{2m\hbar} \int_{\frac{\hbar\ell(\ell+1)}{2mr^2}}^{\omega} \sqrt{\omega - \omega'}\; V_\ell^{-1'}(\hbar\omega')d\omega'\right] .$$

Use integration by parts in the last term and get

$$\delta_\ell(k) = \sqrt{\ell(\ell+1)}\,\frac{\pi}{2} + \lim_{r \to \infty} \left[-kr - \sqrt{2m\hbar}\,\left\{- \sqrt{\frac{\hbar}{2m}}\, \sqrt{k^2 - \frac{\ell(\ell+1)}{r^2}}\, \frac{r}{\hbar} + \frac{1}{2\hbar} \int_{\frac{\hbar\ell(\ell+1)}{2mr^2}}^{\omega} \frac{V_\ell^{-1}(\hbar\omega')d\omega'}{\sqrt{\omega - \omega'}} \right\}\right]$$

$$= \sqrt{\ell(\ell+1)}\,\frac{\pi}{2} - \sqrt{\frac{m}{2\hbar}} \int_{0}^{\omega} \frac{V_\ell^{-1}(\hbar\omega')d\omega'}{\sqrt{\omega - \omega'}} .$$

This gives us the fundamental form for the scattering phase shift in the W.K.B. approximation

$$\delta_\ell(k) = \sqrt{\ell(\ell+1)}\,\frac{\pi}{2} - \sqrt{\frac{m}{2\hbar}} \int_0^\omega \frac{V_\ell^{-1}(\hbar\omega')d\omega'}{\sqrt{\omega-\omega'}} .$$

Notice that this expression also holds for $\ell = 0$, and $\delta_0(k)$ as given by this expression coincides with the same value obtained earlier. A crude estimate for $\delta_\ell(k)$ can be made assuming $-V_\ell^{-1'}(\hbar\omega')$ contributes the largest values for ω' near zero. Doing this we get $\delta_\ell(k) = \sqrt{\ell(\ell+1)}\,\frac{\pi}{2} - kV_\ell^{-1}(\hbar\omega)$, or by multiplying the last term by a factor in order to get $\delta_\ell(k) = 0$ for $V(r) = 0$ we have

$$\delta_\ell(k) \approx \frac{\pi}{2}\left(\sqrt{\ell(\ell+1)} - kV_\ell^{-1}(\hbar\omega)\right) .$$

Inversion of the Expression for $\delta_\ell(k)$

Let us consider the expression

$$\delta_\ell(k) = \sqrt{\ell(\ell+1)}\,\frac{\pi}{2} - \sqrt{\frac{m}{2\hbar}} \int_0^\omega \frac{V_\ell^{-1}(\hbar\omega')d\omega'}{\sqrt{\omega-\omega'}} .$$

It can be rewritten as

$$\delta_\ell(k) = \sqrt{\frac{m}{2\hbar}} \int_0^\omega \frac{\sqrt{\frac{\hbar\ell(\ell+1)}{2m\omega'}} - V_\ell^{-1}(\hbar\omega')]d\omega'}{\sqrt{\omega-\omega'}}$$

This can be inverted as before by using the Abel formula. We observe that the $\delta_\ell(k)$ are not all independent. If $\delta_\ell(k)$ is specified, $V(r)$ is determined, and so therefore is $\delta_\ell(k)$ for each ℓ. If measured values of $\delta_\ell(k)$ are not self-consistent it means that the scattering interaction involves more than just a simple potential. The differential scattering cross section $\frac{d\sigma}{d\Omega} = |f_k(\theta)|^2$ measures the magnitude of $f_k(\theta)$ and the time delay can be used to determine its phase. With $f_k(\theta)$ explicitly known, the scattering phase shifts can be determined from the formula

$$f_k(\theta) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1) e^{i\delta_\ell(k)} \sin \delta_\ell(k) P_\ell(\cos\theta)$$

from which we get

$$e^{i\delta_\ell(k)} \sin \delta_\ell(k) = \frac{k}{2} \int_0^\pi f_k(\theta)\, P_\ell(\cos\theta) \sin\theta d\theta \; .$$

Such a simple method for obtaining the phase shifts $\delta_\ell(k)$ for scattering would not be possible if only $|f_k(\theta)|$ was known and the phase of the scattering amplitude was undetermined. For $e^{i\eta_k(\theta)} = \frac{f_k(\theta)}{|f_k(\theta)|}$ we we have (taking real and imaginary parts above)

$$\cos\delta_\ell(k) \sin\delta_\ell(k) = \frac{k}{2} \int_0^\pi |f_k(\theta)| \cos\eta_k(\theta) P_\ell(\cos\theta) \sin\theta d\theta \; ,$$

$$\sin^2\delta_\ell(k) = \frac{k}{2} \int_0^\pi |f_k(\theta)| \sin\eta_k(\theta) P_\ell(\cos\theta) \sin\theta d\theta \; .$$

Since $\eta_k(\theta) \to n\pi$ as $k \to \infty$ (in the Born approxiamtion) we have $\eta_k(\theta)$ can be found explicitly from the time delay as

$$\eta_k(\theta) = -\frac{\hbar}{m}\int_k^\infty \partial t(k,\theta)k\,dk + n\pi . \qquad \left(\int_0^\infty V(r)dr \ll \hbar v\right)$$

Optical Theorem and Total Scattering Cross Section

From $f_k(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_\ell(k)}\sin\delta_\ell(k)\,P_\ell(\cos\theta)$ we can evaluate the total scattering cross section $\sigma = \int \frac{d\sigma}{d\Omega}d\Omega$ where $\frac{d\sigma}{d\Omega} = |f_k(\theta)|^2$. The result is

$$\sigma = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell(k) \quad .$$

Also $f_k(0) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_\ell(k)}\sin\delta_\ell(k)$ since $P_\ell(1) = 1$. Hence $\frac{4\pi}{k}\operatorname{Im}(f_k(0)) = \sigma$. This result is known as the optical theorem, and it gives an expression for the total scattering cross section σ as a function of k in terms of the scattering amplitude.

The Separable Radial Potential

In the radial Schrödinger equation $U''_{\omega\ell}(r) + (k^2 - \frac{\ell(\ell+1)}{r^2})U_{\omega,\ell}(r) = \frac{2m}{\hbar^2}V(r)U_{\omega\ell}(r)$, and in the corresponding integral equation

$$U_{\omega\ell}(r) = 2rj_\ell(kr) + \frac{2m}{\hbar^2}\int_0^\infty G_\ell(r,s)V(s)U_{\omega\ell}(s)ds$$

it is possible to replace the potential $V(r)$ by an operator on functions of r so $V(r)U_{\omega\ell}(r)$ becomes $\int_0^\infty V(r,s)U_{\omega\ell}(s)ds$. This is the non-local radial potential. For such a potential, the three dimensional Schrödinger equation is

$$i\hbar \frac{\partial\psi}{\partial t}(\vec{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) + \int_0^\infty \frac{s}{r} V(r,s)\psi(s\hat{r},t)ds$$

where $\vec{r} = r\hat{r}$ and $|\vec{r}| = r$.

We are especially interested in those potentials $V(r,s)$ which can be factored as $V(r,s) = V_1(r)V_2(s)$. Such a potential is said to be separable.

From the integral equation for $U_{\omega\ell}(r)$ we have (taking $V_1 = V_2$ and $V(r,s) = V(r)V(s)$),

$$U_{\omega\ell}(r) = 2rj_\ell(kr) + \frac{2m}{\hbar^2}\int_0^r G_\ell(r,s)V(s)ds \int_0^\infty V(q)U_{\omega\ell}(q)dq$$

$$+ \frac{2m}{\hbar^2}\int_r^\infty G_\ell(r,s)V(s)ds \int_0^\infty V(q)U_{\omega\ell}(q)dq \quad ,$$

or

$$U_{\omega\ell}(r) = 2rj_\ell(kr) - \frac{2mirk}{\hbar^2} h_\ell^{(1)}(kr)\ N \int_0^r s\ j_\ell(ks)V(s)ds$$

$$- \frac{2mirk}{\hbar^2} j_\ell(kr)\ N \int_r^\infty s\ h_\ell^{(1)}(ks)V(s)ds \quad ,$$

where

$$N_\ell(k) = \int_0^\infty V(q)U_{\omega\ell}(q)dq \quad .$$

The equation above is an explicit solution for $U_{\omega\ell}(r)$ if N is known. N can be obtained by multiplying the equation for $U_{\omega\ell}(r)$ by $V(r)$, integrating over r from zero to infinity and solving form N. (Since $V(s)$ is assumed to be known.) Let us consider the separable delta function potential $V(r,s) = V(r)V(s) = V_0^2\,\delta(r-a)\delta(s-a)$ so $V(s) = V_0\,\delta(s-a)$. In this case $N = V_0\,U_{\omega\ell}(a)$. We can evaluate $U_{\omega\ell}(r)$ in two cases $r < a$ and $r > a$ to get

$$U_{\omega\ell}(r) = 2rj_\ell(kr) - \frac{2mirk}{\hbar^2}\,j_\ell(kr)V_0U_{\omega\ell}(a)ah_\ell^{(1)}(ka)V_0 \quad \text{for} \quad r < a\,,$$

$$= 2rj_\ell(kr) - \frac{2mirk}{\hbar^2}\,h_\ell^{(1)}(kr)V_0U_{\omega\ell}(a)\,aj_\ell(ka)V_0 \quad \text{for} \quad r > a.$$

If we set $r = a$ we can solve for $U_{\omega\ell}(a)$ to get

$$U_{\omega\ell}(a) = \frac{2aj_\ell(ka)}{1 + 2mia^2V_0^2\,\frac{k}{\hbar^2}\,j_\ell(ka)h_\ell^{(1)}(ka)}\,.$$

Recall that for $r > a$, $U_{\omega\ell}(r) = 2rj_\ell(kr) + \alpha_\ell(\omega)rh_\ell^{(1)}(kr)$.

Hence $\alpha_\ell(\omega) = -\frac{2mik}{\hbar^2}\,aV_0^2\,U_{\omega\ell}(a)j_\ell(ka)$.

For the more general separable potential we can still obtain

$\alpha_\ell(\omega) = -\frac{2mik}{\hbar^2}\,N\int_0^\infty s\,j_\ell(ks)V(s)ds$ where $N = \int_0^\infty V(q)U_{\omega\ell}(q)dq$. This transformation is of interest because it can be inverted. The Spherical Bessel transform or Hankel transform is defined by the equations

$$g(r) = \sqrt{\frac{2}{\pi}}\int_0^\infty j_\ell(kr)f(k)k^2dk \quad \text{and} \quad f(k) = \sqrt{\frac{2}{\pi}}\int_0^\infty j_\ell(kr)g(r)r^2dr\,.$$

Thus we can solve for $V(s)$ in terms of $\alpha_\ell(\omega)$ to obtain

$$V(r) = \frac{ri\hbar^2}{\pi m} \int_0^\infty j_\ell(kr)\,\alpha_\ell\!\left(\frac{\hbar k^2}{2m}\right)\frac{kdk}{N_\ell(k)} .$$

Thus for the separable potential $V(r,s) = V(r)V(s)$ we can obtain the potential factor $V(r)$ form $\alpha_\ell(\omega)$ or from the phase shifts $\delta_\ell(k)$ where $e^{2i\delta_\ell(k)} = 1 + \alpha_\ell(\omega)$. As in the case of a local potential, the phase shifts for a separable potential satisfies a consistency relationship. If $\delta_0(k)$ is specified for all k, all phase shifts $\delta_\ell(k)$ are known. In the case of the separable potential, unlike the local potential, the expression for $V(r)$ is exact and not an approximation. In particular $V(r)$ can be explicitly determined from the s-wave phase shift as

$$V(r) = \frac{i\hbar^2}{\pi m} \int_0^\infty \frac{\sin (kr)}{N_0(k)}\, \alpha_0\!\left(\frac{\hbar k^2}{2m}\right)dk .$$

The usefulness is limited because the dependence of N on k is not known in general unless V is known.

If we consider $V(r,s) = V_1(r)V_2(s)$ where V_1 and V_2 are not necessarily the same we have $N_\ell(k) = \int_0^\infty V_2(q)U_{\omega\ell}(q)dq$, with

$$U_{\omega\ell}(r) = 2rj_\ell(kr) - \frac{2mirk}{\hbar^2} h_\ell^{(1)}(kr)N_\ell(k) \int_0^r s\, j_\ell(ks)V_1(s)ds$$

$$- \frac{2mirk}{\hbar^2} j_\ell(kr)N_\ell(k) \int_r^\infty s\, h_\ell^{(1)}(ks)V_1(s)ds ,$$

and

$$\alpha_\ell(\omega) = -\frac{2mik}{\hbar^2} N_\ell(k) \int_0^\infty s\, j_\ell(ks)V_1(s)ds \quad ,$$

$$V_1(r) = \frac{ir\hbar^2}{\pi m} \int_0^\infty j_\ell(kr)\alpha_\ell(\frac{\hbar k^2}{2m}) \frac{kdk}{N_\ell(k)} \quad .$$

Suppose that $\alpha_\ell(\omega) = 0$ for all ω and some fixed ℓ. Then $U_{\omega\ell}(r) = 2rj_\ell(kr)$ since $N(k) = 0$ and this would imply

$$0 = N_\ell(k) = \int_0^\infty V_2(q)U_{\omega\ell}(q)dq = 2\int_0^\infty V_2(r)rj_\ell(kr)dr \quad .$$

This means $V_2(r) = 0$ by the Hankel Transform. Hence for a non-zero separable potential for every ℓ there exists a k for which $\delta_\ell(k) \neq 0$. The only transparent separable potential is the zero potential.

Discussion of Transparent Potentials

Let us see if there exist any potentials $V(r,s)$ so that if we solve the equation

$$U_{\omega\ell}(r) = 2rj_\ell(kr) + \frac{2m}{\hbar^2}\int_0^\infty G_\ell(r,s)[\int_0^\infty V(s,q)U_{\omega\ell}(q)dq]ds$$

we get the simple solution $U_{\omega\ell}(r) = 2rj_\ell(kr)$ so that $\alpha_\ell(\omega) = 0$. For this to happen we must have

$$0 = \int_0^\infty G_\ell(r,s)[\int_0^\infty V(s,q)qj_\ell(kq)dq]ds$$

at least holding for large r (in the region of phase shift measurement).

Since such $r > s$, where s is in the range of the potential, we can replace $G_\ell(r,s)$ by $G_\ell(r,s) = irskh_\ell^{(1)}(kr)j_\ell(ks)$. Hence we require

$$0 = \int_0^\infty sj_\ell(ks)[\int_0^\infty V(s,q)qj_\ell(kq)dq]ds \quad .$$

Since this holds for all k by the Hankel transform inversion we have $0 = \int_0^\infty V(s,q)qj_\ell(kq)dq$. Again by the Hankel transform inversion $0 = V(s,q)$. Thus there are no non-zero radially symmetric potentials with $\delta_\ell(k) = 0$ for all k and any given ℓ.

THEOREM. Let $\delta_\ell^{(1)}(k)$ be the phase shifts associated with the potential $V^{(1)}(r,s)$ and $\delta_\ell^{(2)}(k)$ be the phase shifts associated with $V^{(2)}(r,s)$. Suppose that for some non-negative integer ℓ_0, $\delta_{\ell_o}^{(1)}(k) = \delta_{\ell_o}^{(2)}(k)$ for all $k \geq 0$. Then $V^{(1)}(r,s) \equiv V^{(2)}(r,s)$ as an operator identity on the scattering states.

Proof. For simplicity we write the integral equations as operator equations. Then

$$U_{\omega\ell}^{(1)} = j_\ell + G_\ell V^{(1)} U_{\omega\ell}^{(1)} \qquad \text{and}$$

$$U_{\omega\ell}^{(2)} = j_\ell + G_\ell V^{(2)} U_{\omega\ell}^{(2)} \quad .$$

Since $\delta_{\ell_o}^{(1)} = \delta_{\ell_o}^{(2)}$ we have $\alpha_{\ell_o}^{(1)} = \alpha_{\ell_o}^{(2)}$ and hence since

$$\alpha_\ell(\omega) = -\frac{2mik}{\hbar^2}\int_0^\infty s\, j_\ell(ks) \underbrace{V(s)\, U_{\omega\ell}(s)} ds$$

in the local potential case, we simply can replace $V(s)U_{\omega\ell}(s)$ by an operator on $U_{\omega\ell}$ in the non-local case and so

$$j_{\ell_o} V^{(1)}U^{(1)}_{\omega\ell_o} = j_{\ell_o} V^{(2)}U^{(2)}_{\omega\ell_o} \text{ , since } \alpha^{(1)}_{\ell_o} = \alpha^{(2)}_{\ell_o} .$$

But the integral involving j_ℓ can be inverted as usual and hence

$$V^{(1)}U^{(1)}_{\omega\ell_o} = V^{(2)}U^{(2)}_{\omega\ell_o} .$$

From our integral equations for $U^{(1)}_{\omega\ell}$ and $U^{(2)}_{\omega\ell}$ we get

$$U^{(1)}_{\omega\ell_o} - U^{(2)}_{\omega\ell_o} = G_{\ell_o}(V^{(1)}U^{(1)}_{\omega\ell_o} - V^{(2)}U^{(2)}_{\omega\ell_o}) = 0 .$$

Thus $U^{(1)}_{\omega\ell_o} = U^{(2)}_{\omega\ell_o}$. This means $[V^{(1)} - V^{(2)}]U^{(1)}_{\omega\ell_o} = 0$. This holds for all $\omega > 0$. Completeness of the radial scattering states (provided there are no bound states) implies $V^{(1)} - V^{(2)}$ is the zero operator. Insofar as the scattering states are concerned, $V^{(1)} = V^{(2)}$.

An important corollary of this result is that all information one needs to know about a radial potential, local or non-local is contained in the s wave scattering phase shift $\delta_o(k)$. This corresponds to the classical case for a radial potential in 3 dimensions where we found that the potential was determined by knowing the time delay $\partial t(0,v_o)$ for impact parameter $b = 0$. The s wave phase shift is given by

$$e^{i\delta_o(k)} \sin \delta_o(k) = \frac{k}{2} \int_o^\pi f_k(\theta) \sin \theta d\theta$$

and this is the only quantity one actually needs to measure experimentally Knowing $\frac{d\sigma}{d\Omega} = |f_k(\theta)|^2$ only is not good enough; the phase of $f_k(\theta)$ is essential.

The Forward Scattering Problem

Let us consider the case where $f_k(\theta) = 0$ except in a narrow neighborhood of $\theta = 0$. We ask the question: Is it possible to construct a potential $V(r,s)$ such that $f_k(\theta)$ satisfies this condition for all $k > 0$? The total scattering cross section is $\sigma(k) = \int |f_k(\theta)|^2 \, d\Omega$, and the solution for $f_k(\theta)$ satisfying this condition is $f_k(\theta) = \sqrt{\frac{\sigma(k)\delta(1-\cos\theta)}{\pi}}\, e^{i\eta_k}$. By the optical theorem, $\sigma(k) = \frac{4\pi}{k}\,\mathrm{Im}(f_k(0)) \Longrightarrow \eta_k = 0$. In fact η_k is proportional to the narrow width of the "delta function" in some sense. Hence $\mathrm{Im}\, f_k(\theta) = 0$. But from

$$f_k(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_\ell(k)}\sin\delta_\ell(k)P_\ell(\cos\theta)$$

we get

$$0 = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell(k)P_\ell(\cos\theta)$$

for all θ meaning $\delta_\ell(k) = 0$. Hence $f_k(\theta) = 0$ and so $\sigma(k) = 0$. This means the potential $V(r,s) = 0$ by our theorems.

Three Dimensional Non-Radial and Non-Local Potential

In this case the integral equation for the energy eigenfunctions $\psi_\omega(\vec{r})$ in normalized form is

$$\psi_\omega(\vec{r}) = \frac{1}{2\pi}\sqrt{\frac{m\epsilon}{\hbar}}\; k^{1/2}\, e^{ikz}$$

$$- \frac{m}{2\pi\hbar^2}\int \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}\; V(\vec{r}\,')\psi_\omega(\vec{r}\,')d^3\vec{r}\,' \quad .$$

The asymptotic behavior is

$$\psi_\omega(\vec{r}) \xrightarrow[r\to\infty]{} \frac{1}{2\pi}\sqrt{\frac{m\epsilon}{\hbar}}\; k^{1/2}\left(e^{ikz} + f_k(\hat{r})\,\frac{e^{ikr}}{r}\right) \quad .$$

The scattering amplitude is

$$f_k(\hat{r}) = -\,\frac{mk^{-(1/2)}}{\hbar^2}\sqrt{\frac{\hbar}{m\epsilon}}\int e^{-ik\hat{r}\cdot\vec{r}\,'}\; V(\vec{r}\,')\psi_\omega(\vec{r}\,')d^3\vec{r}\,' \quad .$$

For non-local potentials we replace the terms $V(\vec{r}\,')\psi_\omega(\vec{r}\,')$ by the operator form $V\psi_\omega(\vec{r}\,')$ or $\int V(\vec{r}\,',\vec{s})\psi_\omega(\vec{s})d^3\vec{s}$ everywhere they occur.

From the expression for $f_k(\hat{r})$ above, it is evident that if $V(\vec{r}\,')$ is a local potential, that $f_k(\hat{r})$ will never be identically zero for all k and $\hat{r}$. This follows from the fact that the three dimensional Fourier transform operator is unitary with the full Hilbert space as its domain. The Fourier transform does not send non-zero functions to zero. If V is non-local, we can choose V to annihilate the time domain D under consideration, i.e., $V\psi_\omega(\vec{r}) = 0$ for all $\omega > 0$. Since D is not the entire Hilbert space, we can make V zero on D and non-zero on the orthogonal complement of D. In this case $f_k(\hat{r}) = 0$ for all k and all $\hat{r}$. This potential operator V which is non-local and not radially symmetric, is said to be transparent with respect to the time domain D. It is clear that asymptotically at large r (where all experimental measurements are made) $\psi_\omega(r)$ is the same as the free particle wavefunction

$$\psi_\omega^f(r) = \frac{1}{2\pi} \sqrt{\frac{m\epsilon}{\hbar}}\, k^{1/2}\, e^{ikz} \quad .$$

It is also clear thet no scattering cross section will be found $\frac{d\sigma}{d\Omega} = 0$, and time delay measurement cannot be made since $f_k(\hat{r}) = 0$ and cannot be phased. Since all measurements in any experiment are made outside the potential region, and outside the non-asymptotic region of the wavefunction, this potential cannot be detected at all. However, all is not lost. This non-local potential cannot be spherically symmetric as we saw, so we simply have to rotate the apparatus, and send incident particles in at a different angle. This amounts to changing the time domain from D to D'. If D' is in the non-zero portion of the domain of the operator V, scattering will occur, and $f_k(\hat{r})$ will not be identically zero. To get full information about V we may have to send incident particles in from many different angles. If V maps every time domain D to zero, V is identically zero on all scattering states. Any potential can be detected by appropriate scattering.

Suppose V is transparent with respect to D. Then $V\psi_\omega(\vec{r}\,') = 0$. Substituting into the integral equation for $\psi_\omega(\vec{r}\,)$ we get

$$\psi_\omega(\vec{r}) = \frac{1}{2\pi}\sqrt{\frac{m\varepsilon}{\hbar}}\, k^{1/2}\, e^{ikz}$$

which is the free particle energy eigenfunction. Thus for a transparent potential with respect to a time domain D, the wavefunction is completely uninfluenced by the potential even in the region close to the potential. The general wavefunction with time dependence is expressed as

$$\psi(\vec{r},t) = \int_0^\infty A(\omega)\psi_\omega(\vec{r})\, e^{-i\omega t}\, d\omega$$

in terms of its energy distribution. For any (non-transparent) potential the initial free wavefunction corresponding to $\psi(\vec{r},t)$ before scattering $\psi_I(\vec{r},t) = \int_0^\infty A(\omega)\psi_\omega^f(\vec{r})e^{-i\omega t}\, d\omega$, has the same energy amplitude $A(\omega)$ if phased at a point ahead of the scattering region. The magnitudes are always equal regardless of phasing point.

Suppose the operator V describes a potential that cannot be detected by scattering, that is, V is non-zero only when operating on its own bound states. We can prove that $V \equiv 0$.

Since $V\psi_\omega(\vec{r}) = 0$ for all ω and all time domains D for the incident wave packet, the scattering amplitude is identically zero and $\psi_\omega(\vec{r}) = \psi_\omega^f(\vec{r})$ in each time domain D. Hence $V\psi_\omega^f(\vec{r}) = 0$ for all $\omega > 0$ in each time domain D. But the free energy eigenfunctions $\psi_\omega^f(\vec{r})$ for all time domains, include the exponentials $e^{i\vec{k}\cdot\vec{r}}$ for all $\vec{k}$ and span the complete Hilbert space. Thus $V = 0$. This justifies the statement that every non-zero potential can be detected by scattering.

Recall that the integral equation for the scattering states is

$$\psi_\omega(\vec{r}) = \psi_\omega^f(\vec{r}) - \frac{m}{2\pi\hbar^2}\int \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} V(\vec{r}\,')\psi_\omega(\vec{r}\,')d^3\vec{r}\,'$$

and the scattering amplitude is $f_k(\hat{r})$.

CHAPTER XIII

THE NARROW WAVE PACKET APPROXIMATION IN ONE DIMENSION

Consider a wave packet in one dimension approaching a potential. Suppose that the potential is slowly varying and the wave packet has narrow width which remains narrow for all times at which the (position) wave packet interacts with the potential.

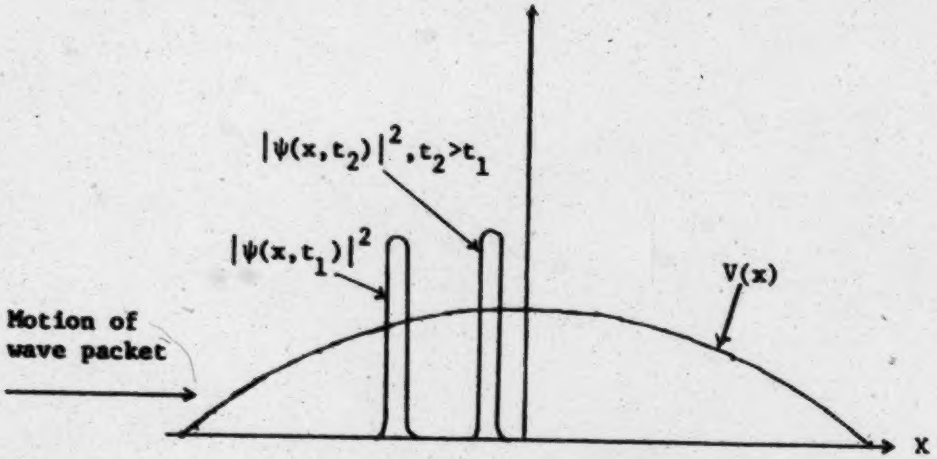

Figure 21

Narrow Wave Packet

We assume that the potential $V(x)$ is essentially constant over the nonzero spread Δx of the wavefunction $\psi(x,t)$ for any fixed t such that $\langle x\rangle_t$ is in the range of the potential. In particular this means we have transmission only, and no reflection. The Schrödinger equation

$i\hbar \frac{\partial\psi}{\partial t}(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}(x,t) + V(x)\,\psi(x,t)$ at any fixed time t can be approximated by replacing $V(x)$ by the constant $V(\langle x\rangle_t) = p(t)$. The constant potential (in x) is accurate over the narrow region of non-zero ψ in position space. Thus we get the new equation

$$i\hbar \frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + p(t)\,\psi \quad .$$

This time separation of variables gives equations which can be explicitly solved in general, unlike the Schrödinger equation. Take $\psi(x,t) = X(x)T(t)$ and get $i\hbar \frac{T'(t)}{T(t)} - p(t) = \hbar\omega$ and $-\frac{\hbar^2}{2m}\frac{X''(x)}{X(x)} = \frac{\hbar^2 k^2}{2m} = \hbar\omega$. Thus $X(x) = e^{ikx}$ and $T(t) = \exp[-\frac{i}{\hbar}\int^t p(s)ds - i\omega t]$. The general approximate solution for $\psi(x,t)$ is a superposition of separable solutions, so that

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} A(k)\, e^{ikx-i\omega t} \exp[-\frac{i}{\hbar}\int^t p(s)ds]\, dk \quad .$$

In terms of the momentum wavefunction

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \phi(k,t_0)\, e^{ikx-i\hbar\frac{k^2}{2m}(t-t_0)} \exp[-\frac{i}{\hbar}\int_{t_0}^{t} p(s)ds]\, dk \quad .$$

Recall that $p(t)$ depends on the particular wave packet chosen, and that Δx the position spread must be small compared to the range of x over which significant variations in $V(x)$ occur for those times t at which $\langle x\rangle_t$ is in the range of the potential. Also note that $p(t) = V(\langle x\rangle_t)$.

Since $\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k,t)\, e^{ikx}\, dk$ we can compare and get

$$\phi(k,t) = \phi(k,t_0)\, e^{-i\hbar \frac{k^2}{2m}(t-t_0)} \exp[- \frac{i}{\hbar} \int_{t_0}^{t} p(s)\, ds] \quad .$$

Since $|\phi(k,t)|^2$ is independent of t, we expect this to be a high energy approximation. From the time dependence of the momentum wavefunction we can get the momentum transformation kernel. We assume $p(s)$ is non zero only for s in some finite interval, and so for $t_0 \to -\infty$, $t \to +\infty$ we have

$$\phi(k,t) = \phi(k,t_0)\, e^{-i\hbar \frac{k^2}{2m}(t-t_0)} \exp[- \frac{i}{\hbar} \int_{-\infty}^{\infty} p(s)\, ds] \quad .$$

For any t', $t_0 \to -\infty$ we have $\phi_1(k',t') = \phi(k',t_0)\, e^{-i\hbar \frac{k'^2}{2m}(t'-t_0)}$. Similarly for any t', $t \to +\infty$ we have $\phi_2(k,t') = \phi(k,t)\, e^{-i\hbar \frac{k^2}{2m}(t'-t)}$. We observe that $\phi_2(k,t') = \int_{-\infty}^{\infty} B_{t'}(k,k')\, \phi_1(k',t')\, dk'$ and so $\phi(k,t)\, e^{-i\hbar \frac{k^2}{2m}(t'-t)} = \int_{-\infty}^{\infty} B_{t'}(k,k')\, \phi(k',t_0)\, e^{-i\hbar \frac{k'^2}{2m}(t'-t_0)}\, dk'$. Substitute $\phi(k,t) = \phi(k,t_0)\, e^{-i\hbar \frac{k^2}{2m}(t-t_0)} \exp[- \frac{i}{\hbar} \int_{-\infty}^{\infty} p(s)\, ds]$ to get $\phi(k,t_0)\, e^{-i\hbar \frac{k^2}{2m}(t'-t_0)} \exp[- \frac{i}{\hbar} \int_{-\infty}^{\infty} p(s) ds] = \int_{-\infty}^{\infty} B_{t'}(k,k')\phi(k',t_0)\, e^{-i\hbar \frac{k'^2}{2m}(t'-t_0)}\, dk'$. For transmission only we have

$B_{t'}(k,k') = \sqrt{2\pi}\, C(k)\, \delta(k-k')$. Substitute above and simplify to get

$$C(k) = \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{i}{\hbar}\int_{-\infty}^{\infty} p_k(s)\, ds\right] \quad .$$

This expression gives the function $C(k)$ which determines the momentum transformation kernel in the narrow wave packet approximation in one dimension. The approximation has lead to an odd result. We expect $C(k)$ to be a function of k but independent of the form of the wave packet. Actually we find $C(k)$ does not depend on k but depends on the function $p(s)$ which is $p(s) = V(\langle x\rangle_{t=s})$ which depends on the average momentum of the wave packet that determines the rate that $\langle x\rangle$ moves through the potential. The subscript k on $p_k(s)$ refers to this average momentum.

Let us now decide what type of function to choose for the initial momentum wave function $\phi_1(k,t)$ which has free particle time dependence. We choose the minimum uncertainty product wave packet we derived earlier, namely

$$\phi_1(k,t) = (2\pi(\Delta k)^2)^{-1/4} \exp(-i\langle x\rangle_{t_1} k - \frac{(k-\langle k\rangle)^2}{4(\Delta k)^2} - \frac{i\hbar k^2}{2m}(t-t_1))$$

where

t_1	is the time of minimum spread of position wavefunction,
$\langle k\rangle$	is the mean (average) or expected momentum (constant in time),
$\langle x\rangle_{t_1}$	is the expected position at time t_1 ,
Δk	is the momentum spread (a constant in time).

The mean (average or expected) energy is $\langle E\rangle = \frac{\hbar^2}{2m}[\langle k\rangle^2 + (\Delta k)^2]$. The position spread Δx at time t is

$$(\Delta x)_t^2 = \frac{1}{4(\Delta k)^2} + \frac{\hbar^2(\Delta k)^2(t-t_1)^2}{2m^2} .$$

Set $t = t_0$ in the expression above for ϕ_1 $(t_0 \to -\infty)$ and use $\phi(k,t) = \phi_1(k,t_0)\, e^{-i\hbar \frac{k^2}{2m}(t-t_0)} \exp[-\frac{i}{\hbar}\int_{-\infty}^{t} p(s)\, ds]$ to get

$$\phi(k,t) = (2\pi(\Delta k)^2)^{-1/4} \exp(-i\langle x\rangle_{t_1} k - \frac{(k-\langle k\rangle)^2}{4(\Delta k)^2} - \frac{i\hbar k^2}{2m}(t-t_1) - i\int_{-\infty}^{t} p(s)ds) ,$$

$$= \phi_1(k,t) \exp[-\frac{i}{\hbar}\int_{-\infty}^{t} p(s)\, ds] .$$

Thus we have the momentum wavefunction $\phi(k,t)$ determined. Including the dependence of $p(s)$ on average momentum we have $\phi(k,t) = \phi_1(k,t) \exp[-\frac{i}{\hbar}\int_{-\infty}^{t} p_k(s)\, ds]$. Now let us evaluate $\langle x\rangle_t = \langle i \frac{\partial}{\partial k}\rangle_t$ on the function $\phi(k,t)$. We are particularly interested in values of $\langle x\rangle_t$ that lie in the range of the potential.

$$\langle x\rangle_t = \int_{-\infty}^{\infty} \phi^*(k,t)[i \frac{\partial}{\partial k}]\, \phi(k,t)\, dk$$

$$= \int_{-\infty}^{\infty} \phi_1^*(k,t)[i \frac{\partial}{\partial k}]\phi_1(k,t)dk + \int_{-\infty}^{\infty} |\phi_1(k,t)|^2 \frac{1}{\hbar} [\int_{-\infty}^{t} \frac{\partial p_k}{\partial k}(s)\, ds]\, dk$$

$$= \langle x\rangle^f_{t_1} + \frac{\hbar}{m}\langle k\rangle(t-t_1) + \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}\ \hbar\Delta k} \exp\left(\frac{-(k-\langle k\rangle)^2}{2(\Delta k)^2}\right)\left[\int_{-\infty}^{t} \frac{\partial p_k}{\partial k}(s)\ ds\right] dk \ .$$

We can integrate by parts in this last expression to get

$$\langle x\rangle_t = \langle x\rangle^f_{t_1} + \frac{\hbar}{m}\langle k\rangle(t-t_1) + \int_{-\infty}^{\infty} \frac{(k-\langle k\rangle)}{\sqrt{2\pi}\ \hbar(\Delta k)^3} \exp\left(\frac{-(k-\langle k\rangle)^2}{2(\Delta k)^2}\right)\left[\int_{-\infty}^{t} p_k(s)ds\right]dk \ .$$

Thus

$$\frac{d}{dt}\langle x\rangle_t = \frac{\hbar}{m}\langle k\rangle + \int_{-\infty}^{\infty} \frac{(k-\langle k\rangle)}{\sqrt{2\underset{\pi}{m}}\ \hbar(\Delta k)^3} \exp\left(-\frac{(k-\langle k\rangle)^2}{2(\Delta k)^2}\right) p_k(t)\ dk$$

$$= \frac{\hbar}{m}\langle k\rangle + \int_{-\infty}^{\infty} |\phi_1(k,t)|^2\ \frac{1}{\hbar}\left(\frac{\partial p_k(t)}{\partial k}\right) dk \ .$$

This gives the deviation of $\langle x\rangle_t$ from the free particle case due to the influence of the potential. Recall the expression we derived for expected time delay for a local potential in one dimension, namely

$$\Delta t(k) = \frac{m\lambda'(k)}{\hbar k} \quad \text{where} \quad \frac{c(k)}{|c(k)|} = e^{i\lambda(k)} \ .$$

Using $c(k) = \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{i}{\hbar}\int_{-\infty}^{\infty} p_k(s)\ ds\right]$ we see that

$$\Delta t(k) = -\frac{m}{\hbar^2 k}\int_{-\infty}^{\infty} \frac{\partial}{\partial k} p_k(s)\ ds \ .$$

Let us examine the conditions needed for the narrow wave approximation to be good. Let us suppose the potential $V(x)$ has range $2a$ (i.e. $V(x) = 0$ for $|x| > a$). Let V_{max} = the maximum value of $|V(x)|$. and suppose that $\frac{|V'(x)|}{V_{max}} \leq k_0$ for some $k_0 > 0$, k_0 finite (i.e. take $k_0 = \frac{1}{V_{max}} \max \left|\frac{dV(x)}{dx}\right|$). Then k_0, $2a$, V_{max} are the three limiting properties of the potential $V(x)$ we wish to consider.

Now let us look at the parameters specifying $\phi_1(k,t)$ and see how these relate to the conditions of the approximation.

(1) Momentum spread $\Delta k > 0$.

(2) Average momentum $(\langle k \rangle) > 0$. We require $(\langle k \rangle) \gg (\Delta k)$ since the incoming wave packet is assumed to have only positive momenta contributing in the superposition.

(3) Time of minimum spread t_1. We set $t_1 = 0$ for convenience.

(4) Expected position at t_1. We take $\langle x \rangle_{t_1} = 0$. This means the free particle achieves its minimum spread at what would normally be the centre of the potential for the potential absent. This is reasonable. We want Δx to be as small as possible in the interaction region.

In estimating the condition on the potential $V(x)$ for the Narrow wave packet approximation to be good, we ignore the effects of the potential itself on the free particle wavefunction $\phi_1(k,t)$. We assume that the free particle wavefunction does very little spreading, and Δx remains at the minimum value (approximately) permitted by uncertainty throughout the passage of the region $-a \leq x \leq a$. We also assume that $\Delta x \ll a$ and

$k_0\ \Delta x << 1$, i.e. $\Delta x << \min\{a\ ,\ \frac{1}{k_0}\}$ and remains so. Recall $(\Delta x)^2_t = \frac{1}{4(\Delta k)^2} + \frac{\hbar^2(\Delta k)^2(t-t_1)^2}{2m^2}$. The spread is a minimum at $t = t_1 = 0$. The wave packet centre is at $\langle x\rangle_{t_2} = a$ at time $t_2 = \frac{ma}{\hbar\langle k\rangle}$. The controlled spreading condition is $\frac{\hbar^2(\Delta k)^2 t_2^2}{2m^2} \le \frac{1}{2(\Delta k)^2}$, or $(\Delta k)^2 \le (\frac{\langle k\rangle}{a})$. The condition $\Delta x << a$ means $(\Delta k)a >> 1$. Also $\frac{k_0}{\Delta k} << 1$ comes from $k_0\ \Delta x << 1$, and of course we had $(\langle k\rangle) >> \Delta k$. Thus $\sqrt{\frac{a}{\langle k\rangle}} \le \frac{1}{\Delta k} << \min\{a\ ,\ \frac{1}{k_0}\}$ and $\frac{1}{\langle k\rangle} << \frac{1}{\Delta k}$. It is easy to see that the parameters a , k_0 , V_{max} of the potential itself must satisfy $k_0 > \frac{1}{a}$ by applying $|V'(x)| \le V_{max}\ k_0$ to a triangular potential with height V_{max} at $x = 0$ and satisfying $V(-a) = V(a) = 0$. Thus $\min\{a\ ,\ \frac{1}{k_0}\} = \frac{1}{k_0}$. Thus $\frac{1}{a} < k_0 << \Delta k \le \sqrt{\frac{\langle k\rangle}{a}} << \langle k\rangle$. Without Δk we have $\frac{1}{a} < k_0 << \sqrt{\frac{\langle k\rangle}{a}} << (\langle k\rangle)$. All these inequalities hold if we merely assume $k_0 << \sqrt{\frac{\langle k\rangle}{a}}$. Since $\frac{1}{a} < k_0$ for any potential, we derive $(\langle k\rangle) >> \frac{1}{a}$ and hence $\sqrt{\frac{\langle k\rangle}{a}} << (\langle k\rangle)$. Thus the only condition we need to impose on $\langle k\rangle$ in order that the narrow wave packet approximation be good is $k_0 << \sqrt{\frac{\langle k\rangle}{a}}$. In addition to this high energy condition, we must also have the momentum spread Δk satisfying $k_0 << \Delta k \le \sqrt{\frac{\langle k\rangle}{a}}$. The condition $(\langle k\rangle) >> k_0^2\, a$ is both necessary and sufficient for the narrow wave packet approximation to be good. If $(\langle k\rangle) >> k_0^2\, a$ simply take $\Delta k = \sqrt{\frac{\langle k\rangle}{a}}$ and construct the free packet $\phi_1(k,t)$ with $t_1 = 0$ and $\langle x\rangle_{t_1} = 0$ according to the formula for the minimum uncertainty momentum wavefunction. In order to insure that the variations in potential over the range of Δx are small compared to the incident energy we require $\frac{\hbar^2\langle k\rangle^2}{2m} \gtrsim V_{max}$, that is we do not have $\frac{\hbar^2\langle k\rangle^2}{2m} << V_{max}$. In fact we require $\frac{\hbar^2\langle k\rangle^2}{2m} > V_{max}$ in order to construct the classical formula for $p_k(t)$ namely

$$p_k(t) = V(\gamma_k(t))$$

where

$$\gamma_k^{-1}(x) = \frac{m}{\hbar k}\int_0^x \frac{dy}{\sqrt{1 - \frac{2mV(y)}{\hbar^2 k^2}}} \ .$$

In this case $x = 0$ when $t = 0$. Let us evaluate $\frac{\partial p_k(t)}{\partial k}$ for constant t . This is given by $\frac{\partial p_k(t)}{\partial k} = V'(x)\,\frac{\partial x}{\partial k}$ where $x = \gamma_k(t)$ and t is constant. From $t = \frac{m}{\hbar k}\int_0^x \frac{dy}{\sqrt{1 - \frac{2mV(y)}{\hbar^2 k^2}}}$ we differentiate with respect to k for constant t to get

$$\frac{\hbar t}{m} = \frac{\partial}{\partial k}\int_0^x \frac{dy}{\sqrt{1 - \frac{2mV(y)}{\hbar^2 k^2}}} = \frac{\frac{\partial x}{\partial k}}{\sqrt{1 - \frac{2mV(x)}{\hbar^2 k^2}}} - \frac{2m}{\hbar^2 k^3}\int_0^x \frac{V(y)\,dy}{(1 - \frac{2mV(y)}{\hbar^2 k^2})^{3/2}} \ .$$

Thus

$$\frac{\partial x}{\partial k} = \frac{\hbar t}{m}\sqrt{1 - \frac{2mV(x)}{\hbar^2 k^2}} + \frac{2m}{\hbar^2 k^3}\sqrt{1 - \frac{2mV(x)}{\hbar^2 k^2}}\int_0^x \frac{V(y)\,dy}{(1 - \frac{2mV(y)}{\hbar^2 k^2})^{3/2}} \ .$$

Hence

$$\frac{\partial p_k(t)}{\partial k} = \frac{\hbar t}{m}\sqrt{1-\frac{2mV(x)}{\hbar^2k^2}}\,V'(x) + \frac{2m}{\hbar^2k^3}\sqrt{1-\frac{2mV(x)}{\hbar^2k^2}}\int_0^x \frac{V(y)\,dy}{\left(1-\frac{2mV(y)}{\hbar^2k^2}\right)^{3/2}}\,V'(x) .$$

We will consider evaluating $\int_{-\infty}^{\infty}[\frac{\partial}{\partial k}p_k(t)]\,dt$. Having evaluated $\frac{\partial p_k(t)}{\partial k}$ at constant t, we multiply it by $\frac{dt}{dx}dx$ where $\frac{dt}{dx}$ is taken at constant k and equals $\frac{m}{\hbar k\sqrt{1-\frac{2mV(x)}{\hbar^2k^2}}}$. Hence $\frac{\partial p_k(t)}{\partial k}dt = \frac{t}{k}V'(x)\,dx + \frac{2m^2V'(x)dx}{\hbar^3k^4}\int_0^x \frac{V(y)dy}{\left(1-\frac{2mV(y)}{\hbar^2k^2}\right)^{3/2}}$, and so

$$\frac{\partial p_k(t)}{\partial k}dt = \frac{m}{\hbar k^2}V'(x)dx\int_0^x \frac{dy}{\sqrt{1-\frac{2mV(y)}{\hbar^2k^2}}} + \frac{2m^2V'(x)dx}{\hbar^3k^4}\int_0^x \frac{V(y)\,dy}{\left(1-\frac{2mV(y)}{\hbar^2k^2}\right)^{3/2}} .$$

Now integrate both sides. The two terms on the right hand side can each be integrated by parts. The limits on x may be taken as $-a$ to a or $-\infty$ to ∞. In either case $V(x)$ vanishes at both limits and so there are no boundary terms in the partial integrations. Hence

$$\int_{-\infty}^{\infty}\frac{\partial p_k(t)}{\partial k}dt = -\frac{m}{\hbar k^2}\int_{-a}^{a}\frac{V(x)dx}{\sqrt{1-\frac{2mV(x)}{\hbar^2k^2}}} - \frac{2m^2}{\hbar^3k^4}\int_{-a}^{a}\frac{[V(x)]^2\,dx}{\left(1-\frac{2mV(x)}{\hbar^2k^2}\right)^{3/2}} .$$

From $\Delta t(k) = -\frac{m}{\hbar^2k}\int_{-\infty}^{\infty}\frac{\partial}{\partial k}p_k(t)\,dt$ we get

$$\Delta t(k) = \frac{m^2}{\hbar^3 k^3} \int_{-a}^{a} \frac{V(x)\,dx}{\sqrt{1 - \frac{2mV(x)}{\hbar^2 k^2}}} + \frac{2m^3}{\hbar^5 k^5} \int_{-a}^{a} \frac{[V(x)]^2\,dx}{(1 - \frac{2mV(x)}{\hbar^2 k^2})^{3/2}}$$

$$= \frac{m^2}{\hbar^3 k^3} \int_{-a}^{a} \frac{[(1 - \frac{2mV(x)}{\hbar^2 k^2})V(x) + \frac{2m}{\hbar^2 k^2}[V(x)]^2]\,dx}{(1 - \frac{2mV(x)}{\hbar^2 k^2})^{3/2}}$$

$$= \frac{m^2}{\hbar^3 k^3} \int_{-a}^{a} \frac{V(x)\,dx}{(1 - \frac{2mV(x)}{\hbar^2 k^2})^{3/2}} .$$

Let us look again more closely at the approximation conditions. The spreading condition on Δx in the range of the potential was derived by replacing the potential itself by a free particle. We have no idea what effect this has on the approximating conditions. It turns out that the condition $\frac{\hbar^2 \langle k \rangle^2}{2m} \gtrsim V_{max}$ will have to be replaced by $\frac{\hbar^2 \langle k \rangle^2}{2m} \gg V_{max}$. The first hint of this appears in the time delay expression

$\Delta t = \frac{m^2}{\hbar^3 k^3} \int_{-a}^{a} \frac{V(x)\,dx}{(1 - \frac{2mV(x)}{\hbar^2 k^2})^{3/2}}$ which agrees with classical time delay

$\Delta t = \frac{m}{\hbar k} \int_{-a}^{a} \frac{dx}{\sqrt{1 - \frac{2mV(x)}{\hbar^2 k^2}}} - \frac{2ma}{\hbar k}$ in the $\frac{1}{k^3}$ term of the expansion, but differs in the $\frac{1}{k^5}$ term. The best way to show the breakdown of the narrow wave packet approximation for low energies $\frac{\hbar^2 \langle k \rangle^2}{2m}$ near V_{max} is to consider total energy. Recall that the momentum wavefunction in the narrow wave packet approximation is

$\phi(k,t) = \phi_1(k,t) \exp [-\frac{i}{\hbar}\int_{-\infty}^{t} P_k(s)\, ds]$. The expected value of total energy $\langle E\rangle = \frac{\hbar^2}{2m}[\langle k\rangle^2 + (\Delta k)^2] \approx \frac{\hbar^2\langle k\rangle^2}{2m}$ since $\Delta k \ll (\langle k\rangle)$. For any time t , $\langle E\rangle = \langle\frac{\hbar^2k^2}{2m}\rangle_t + \langle V(x)\rangle_t$. Now

$$\langle\frac{\hbar^2k^2}{2m}\rangle_t = \frac{\hbar^2}{2m}\int |\phi(k,t)|^2\, k^2 dk = \frac{\hbar^2}{2m}\int |\phi_1(k,t)|^2\, k^2\, dk$$

$$= \langle\frac{\hbar^2k^2}{2m}\rangle^{f} = \langle E\rangle = \frac{\hbar^2}{2m}[\langle k\rangle^2 + (\Delta k)^2] \quad .$$

This gives us $\langle V(x)\rangle_t = 0$ so clearly this is not much of a potential. To give a consistent approximation, $\langle V(x)\rangle_t \ll \frac{\hbar^2\langle k\rangle^2}{2m}$. For a narrow wave packet $\langle V(x)\rangle_t \approx V(\langle x\rangle_t) = P_{\langle k\rangle}(t)$. The approximation is guaranteed for $V_{max} \ll \frac{\hbar^2\langle k\rangle^2}{2m}$. Observe that

$$i\hbar\frac{\partial\phi(k,t)}{\partial t} = \frac{\hbar^2k^2}{2m}\phi(k,t) + P_k(t)\,\phi(k,t)$$

is the differential equation satisfied by $\phi(k,t)$ in the narrow wave packet approximation. If we multiply by $\phi^*(k,t)$ and integrate over k we get

$$\langle i\hbar\frac{\partial}{\partial t}\rangle = \langle\frac{\hbar^2k^2}{2m}\rangle + \int_{-\infty}^{\infty} |\phi(k,t)|^2\, P_k(t)\, dk$$

$$= E + \int_{-\infty}^{\infty} |\phi(k,t)|^2\, P_k(t)\, dk \approx E \quad .$$

E is constant, and $\int_{-\infty}^{\infty} |\phi(k,t)|^2 \, P_k(t) \, dk \ll E$.

Like the Born approximation, this is a high energy weak potential approximation and not semi-classical. For a more complicated semi-classical treatment of narrow wave packets see Lebedeff.

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APPENDIX I

THE HERMITE EXPANSION FUNCTIONS

The Hermite expansion functions are $\psi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x) e^{-x^2/2}$. If F represents the Fourier transform operator defined by $(Ff)(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(k) e^{ikx} dk$ then $F\psi_n = i^n \psi_n$ and $F^{-1} \psi_n = (-i)^n \psi_n$. With respect to the basis $\begin{bmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix}$, F is an infinite dimensional diagonal matrix with i^n in the nth diagonal position. (The initial position corresponds to $n = 0$ and not $n = 1$.) Clearly F is a unitary transformation. If we represent the function $f(x) = \sum_{n=0}^{\infty} f_n \psi_n(x)$ by the column vector $\begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix}$, the Fourier transform of f is $\begin{bmatrix} f_0 \\ if_1 \\ -f_2 \\ -if_3 \\ \cdot \\ \cdot \end{bmatrix}$. We represent linear operators by infinite dimensional matrices and functions by column vectors in this system.

Some of the properties of $\psi_n(x)$ are the following.

$$\psi_n(x) = (-1)^n \psi_n(-x) \quad ,$$

$$(x + \frac{d}{dx})\, \psi_n(x) = \sqrt{2n}\, \psi_{n-1}(x) \quad ,$$

$$(x - \frac{d}{dx})\, \psi_n(x) = \sqrt{2(n+1)}\, \psi_{n+1}(x) \quad ,$$

$$x\, \psi_n(x) = \sqrt{\frac{n}{2}}\, \psi_{n-1}(x) + \sqrt{\frac{n+1}{2}}\, \psi_{n+1}(x) \quad ,$$

$$\frac{\partial \psi_n}{\partial x}(x) = \sqrt{\frac{n}{2}}\, \psi_{n-1}(x) - \sqrt{\frac{n+1}{2}}\, \psi_{n+1}(x) \quad ,$$

$$\int_{-\infty}^{\infty} \psi_n(x)\, \psi_m(x)\, dx = \delta_{nm} \quad .$$

If $f(x) = \sum_{n=0}^{\infty} f_n\, \psi_n(x)$ then $f_n = \int_{-\infty}^{\infty} f(x)\, \psi_n(x)\, dx$. Also we have the formal expansion

$$\delta(x-x_0) = \sum_{n=0}^{\infty} \psi_n(x_0)\, \psi_n(x) \quad ,$$

$$\frac{1}{\sqrt{2\pi}}\, e^{ikx} = \sum_{n=0}^{\infty} \psi_n(k)\, i^n \psi_n(x) \quad .$$

Summation and Integration Conventions.

There are two types of variable used in this analysis, discrete and continuous. A discrete variable takes on only the values 0,1,2,3,4,... and a continuous variable takes on any real value. If a symbol representing a discrete or continuous variable appears on both sides of an equation, it is understood that the expression of equality holds for all allowable values of the variable. If a discrete variable appears on one side of an equation only it is understood that a sum from 0 to ∞ is taken on the term containing this variable. If a continuous variable appears on one side of an equation only, it is understood that the term containing this variable is integrated from $-\infty$ to ∞ with respect to that symbol.

As examples of the above conventions we have

$$(-i)^n \psi_n(x) = \frac{1}{\sqrt{2\pi}} \psi_n(k)\, e^{-ikx} \quad ,$$

$$i^n \psi_n(x) = \frac{1}{\sqrt{2\pi}} \psi_n(k)\, e^{ikx} \quad ,$$

$$f(x) = f_n \psi_n(x) \quad \text{and} \quad f_n = f(x)\psi_n(x) \quad ,$$

$$\delta(x-x_0) = \psi_n(x_0)\psi_n(x) \quad \text{and} \quad \frac{1}{\sqrt{2\pi}} e^{ikx} = \psi_n(k) i^n \psi_n(x) \quad .$$

The recursion expressions for evaluating ψ_n are

$$\psi_0(x) = \pi^{-1/4} e^{-x^2/2} \quad , \quad \psi_1(x) = \sqrt{2}\, x\, \psi_0(x)$$

and

$$\psi_{n+1}(x) = \frac{\sqrt{2}\, x\, \psi_n(x) - \sqrt{n}\, \psi_{n-1}(x)}{\sqrt{n+1}} \qquad \text{for} \quad n = 1,2,3,\ldots \quad .$$

The Hermite polynomials $H_n(x)$ which are used to define $\psi_n(x)$ satisfy the following conditions.

$$H_n''(t) - 2t\, H_n'(t) + 2n\, H_n(t) = 0 \quad ,$$

$$H_n(t) = \sum_{r=0}^{\frac{1}{2} n \text{ or } \frac{1}{2}(n-1)} \frac{(-1)^r\, 2^{n-2r}\, n!\, t^{n-2r}}{(n-2r)!\; r!} \quad ,$$

$$H_n'(t) = 2n\, H_{n-1}(t) \quad , \quad H_n(x) = 2x\, H_{n-1}(x) - 2(n-1)\, H_{n-2}(x) \quad ,$$

$$e^{-s^2+2sx} = \sum_{n=0}^{\infty} \frac{H_n(x) s^n}{n!} \quad , \quad \int_{-\infty}^{\infty} e^{-x^2}\, H_n(x)\, H_m(x) dx = 2^n\, n! \sqrt{\pi}\, \delta_{nm} \quad ,$$

$$H_n(x) = \frac{d^n}{ds^n} [e^{x^2-(s-x)^2}]_{s=0} = (-1)^n\, e^{x^2}\, \frac{d^n}{dx^n}\, e^{-x^2}$$

$$= e^{x^2/2}\, (x - \frac{d}{dx})^n\, e^{-x^2/2} \quad ,$$

$$\int_{-\infty}^{\infty} e^{-(x-s)^2}\, H_n(x) = dx = \int_{-\infty}^{\infty} e^{-x^2}\, H_n(s+x) dx = (2s)^n \sqrt{\pi} \quad .$$

The differential equation for $\psi_n(x)$ can be obtained by applying $(x + \frac{d}{dx})(x - \frac{d}{dx})$ and is given by

$$\frac{d^2\, \psi_n}{dx^2} + (2n+1 - x^2)\psi_n = 0 \quad .$$

The delta function $\delta(x-x_0)$ is given by $\delta(x-x_0) = \sum_{n=0}^{\infty} \psi_n(x)\psi_n(x_0)$. From this we can show that $\delta(x-x_0)$ is an eigenfunction of the operator x with eigenvalue x_0 , that is $x\delta(x-x_0) = x_0\delta(x-x_0)$.

Proof:

$$x\delta(x-x_0) = \sum_{n=0}^{\infty} \psi_n(x_0)x\psi_n(x)$$

$$= \sum_{n=0}^{\infty} \psi_n(x_0)\left[\sqrt{\frac{n}{2}}\,\psi_{n-1}(x) + \sqrt{\frac{n+1}{2}}\,\psi_{n+1}(x)\right]$$

$$= \sum_{n=1}^{\infty} \psi_n(x_0)\sqrt{\frac{n}{2}}\,\psi_{n-1}(x) + \sum_{n=0}^{\infty} \psi_n(x_0)\sqrt{\frac{n+1}{2}}\,\psi_{n+1}(x)$$

$$= \sum_{n=0}^{\infty} \psi_{n+1}(x_0)\sqrt{\frac{n+1}{2}}\,\psi_n(x) + \sum_{n=0}^{\infty} \psi_{n-1}(x_0)\sqrt{\frac{n}{2}}\,\psi_n(x)$$

$$= \sum_{n=0}^{\infty} \left[\sqrt{\frac{n+1}{2}}\,\psi_{n+1}(x_0) + \sqrt{\frac{n}{2}}\,\psi_{n-1}(x_0)\right]\psi_n(x)$$

$$= \sum_{n=0}^{\infty} [x_0\psi_n(x_0)]\,\psi_n(x) = x_0\delta(x-x_0) \quad .$$

Notice that the sums above are divergent as they stand and each term is understood to represent the kernel $k(x,x_0)$ of some operator on a class of functions which allows the sums to converge.

As a special case of the above result we get $x\delta(x) = 0$. This can be used to determine properties of the derivative of the delta function. Aside from the important result

$$f^{[n]}(x) = (-1)^n \int_{-\infty}^{\infty} f(x_0)\ \delta^{[n]}(x_0-x)\ dx_0$$

where $[n]$ denotes nth derivative, we can obtain by differentiating $x\delta(x) = 0$, the equation

$$x^k \delta^{[n]}(x) = (-1)^k \frac{n!}{(n-k)!} \delta^{[n-k]}(x) \quad , \quad \text{for} \quad n \geq k$$

$$= 0 \qquad\qquad \text{for} \quad n < k \quad .$$

We can use this result to obtain information about a class of functions we call delspan or general. First of all observe an important analogy about raising and lowering operators, orthogonal, analytic and general or delspan representations of a function (or generalized function).

Three classes of function (operator) expansions are given below.

TABLE II

FUNCTION EXPANSIONS

	Orthogonal	Analytic	General or Delspan
Function Expansion	$f(x) = \sum_{n=0}^{\infty} f_n \psi_n(x)$	$g(x) = \sum_{n=0}^{\infty} g_n x^n$	$h(x) = \sum_{n=0}^{\infty} h_n \delta^{[n]}(x)$
Coefficient Inversion	$f_n = \int_{-\infty}^{\infty} f(x)\psi_n(x)\,dx$	$g_n = \frac{g^{[n]}(0)}{n!}$	$h_n = \frac{(-1)^n}{n!}\int_{-\infty}^{\infty} x^n h(x)\,dx$
Raising Operator	$(x - \frac{d}{dx})\psi_n(x) = \sqrt{2(n+1)}\,\psi_{n+1}(x)$	$xx^n = x^{n+1}$	$\frac{d}{dx}\delta^{[n]}(x) = \delta^{[n+1]}(x)$
Lowering Operator	$(x + \frac{d}{dx})\psi_n(x) = \sqrt{2n}\,\psi_{n-1}(x)$	$\frac{d}{dx} x^n = n\, x^{n-1}$	$x\delta^{[n]}(x) = -n\delta^{[n-1]}(x)$.

As an additional result we have the exponential expansions

$$\frac{e^{ikx}}{\sqrt{2\pi}} = \sum_{n=0}^{\infty} \psi_n(k)\ i^n\ \psi_n(x)$$

$$e^{ikx} = \sum_{n=0}^{\infty} \frac{i^n}{n!} k^n\ x^n$$

$$\frac{e^{ikx}}{2\pi} = \sum_{n=0}^{\infty} \frac{i^n}{n!} \delta^{[n]}(k)\ \delta^{[n]}(x) \quad .$$

The first two we know already, while the last one is proved later.

Fourier Transform of a General Function

Let $g(x) = \sum_{n=0}^{\infty} b_n\ \delta^{[n]}(x)$ be general with expansion coefficients $b_n = \frac{(-1)^n}{n!} \int_{-\infty}^{\infty} x^n\ g(x)dx$. By "function" we really mean linear functional which maps a linear space S of functions into complex or real numbers. If $h \epsilon S$,

$$g(h) = \int_{-\infty}^{\infty} g(x)h(x)dx = \sum_{n=0}^{\infty} (-1)^n\ b_n\ h^{[n]}(0) \quad \text{, a scalar.}$$

The function space S is the largest one which allows all sums and integrals to converge when a given function is explcitly operated on from S . The integrals and sums representing the operator themselves do not necessarily converge.

Let f be the Fourier transform of g , i.e. $f = F\ g$, so

$$f(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(x)\, e^{ikx}\, dx \quad .$$

Thus

$$f(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(x) \sum_{n=0}^{\infty} \frac{(ik)^n\, x^n}{n!}\, dx$$

$$= \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{\infty} (-ik)^n\, b_n = \sum_{n=0}^{\infty} \frac{f^{[n]}(0)}{n!}\, k^n \quad .$$

Hence $f^{(n)}(0) = \dfrac{n!(-i)^n b_n}{\sqrt{2\pi}}$. Thus the Fourier transform of a general function is analytic, and the Fourier transform of an analytic function is general. The orthogonal functions

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}}\, H_n(x)\, e^{-x^2/2}$$

are both analytic and general.

Expanding an Operator

Let $k(x,y) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} k_{nm}\psi_n(x)\, \psi_m(y)$ be the expansion of the kernel of an operator k . If $f(y) = \sum_{n=0}^{\infty} f_n\, \psi_n(y)$ then $kf = g$ where

$$g(x) = \int_{-\infty} k(x,y)f(y)dy = \sum_{n=0}^{\infty} \Big(\sum_{m=0}^{\infty} k_{nm} f_m \Big) \psi_n(x)$$

$$= \sum_{n=0}^{\infty} g_n\, \psi_n(x) \quad .$$

Hence $g_n = k_{nm} f_m$ with summation convention of m. In fact using the summation and integration conventions, we can write the above equations as $k(x,y) = k_{nm}\,\psi_n(x)\,\psi_m(x)$, $f(y) = f_n\,\psi_n(y)$, $f_n = f(y)\,\psi_n(y)$, $g(x) = g_n\,\psi_n(x)$, $g_n = g(x)\,\psi_n(x)$, $g_n = k_{nm}\,f_m$ and $g(x) = k(x,y)\,f(y)$. The equation $g_n = k_{nm}\,f_m$ is the matrix representation of $g(x) = k(x,y)\,f(y)$. The matrix elements are $k_{nm} = k(x,y)\,\psi_n(x)\,\psi_m(y)$. The general operator equation is $kf = g$.

Consider the operator $A_\pm$ defined by $A_\pm = x \pm \frac{d}{dx}$, i.e., if $g = A_\pm f$ then $g(x) = (x \pm \frac{d}{dx})f$. The matrix elements are

$$A_{\pm nm} = \psi_n(x)(x \pm \frac{d}{dx})\,\psi_m(x)\ .$$

This gives $A_{+nm} = \sqrt{2m}\,\delta_{n,m-1}$ and $A_{-nm} = \sqrt{2n}\,\delta_{n,m+1}$. Also

$$A_+(x,y) = \sum_{n=0}^{\infty} \sqrt{2(n+1)}\ \psi_n(x)\psi_{n+1}(y)\ ,$$

$$A_-(x,y) = \sum_{n=0}^{\infty} \sqrt{2(n+1)}\ \psi_{n+1}(x)\psi_n(y)\ .$$

Operator Expansion Relations

Suppose an operator Λ is expanded in the form

$$\Lambda = \sum_{k=0}^{\infty} \sum_{n=0}^{\infty} a_{kn}\, x^k \left(\frac{d}{dx}\right)^n\ .$$

How are the coefficients a_{kn} related to the matrix elements $\Lambda_{nm} = \int \psi_n \Lambda \psi_m$?

Can every operator be expressed in the form shown above for Λ ?

The simplest separable operator has the kernel $E^{(n,m)}(x,y) = \psi_n(x)\,\psi_m(y)$ for some fixed n and m. The matrix elements of $E^{(n,m)}(x,y)$ are $E^{(n,m)}_{\ell s} = \delta_{n\ell}\delta_{ms}$. The operator k with matrix k_{nm} can be expanded in terms of the separable operators as $k = k_{nm}\,E^{(n,m)}$. As a kernel, $k(x,y) = k_{nm}\,E^{(n,m)}(x,y)$ with summation of course. Hence if the separable operators can be expanded in the form shown for Λ, any operator can. The operator Λ can be written in the equivalent form with different coefficients b_{kn} as follows.

$$\Lambda = \sum_{k=0}^{\infty}\sum_{n=0}^{\infty} b_{kn}\left(x - \frac{d}{dx}\right)^k \left(x + \frac{d}{dx}\right)^n \quad . \qquad (*)$$

Clearly, if Λ is expressible as in (*) it can be expanded also in the form

$$\Lambda = \sum_{k=0}^{\infty}\sum_{n=0}^{\infty} a_{kn}\, x^k \left(\frac{d}{dx}\right)^n \quad . \qquad (\dagger)$$

Also linear combinations of operators of the form (*) are also of the form (*). Similarly linear combinations of (†) type operators are (†) type operators. Moreover composition of (†) type operators are (†) type operators. The operators x and $\frac{d}{dx}$ are both of type (*) and (†). If we can prove that compositions of (*) type operators are (*) type operators then we know all (†) operators are (*) operators since every (†) operator is built up of compositions and linear combination of x and $\frac{d}{dx}$ which are (*) operators. It is enough to prove that $(x + \frac{d}{dx})(x - \frac{d}{dx})$ is of type (*). But as operators $(x + \frac{d}{dx})(x - \frac{d}{dx}) = (x - \frac{d}{dx})(x + \frac{d}{dx}) + 2$ and both operators on the right hand side are of type (*). Hence operators of type (*) and type (†) are equivalent.

First of all, observe that

$$(x + \frac{d}{dx})^n \psi_m(x) = 2^{n/2} \sqrt{\frac{m!}{(m-n)!}}\, \psi_{m-n}(x) \quad ,$$

$$(x - \frac{d}{dx})^k \psi_p(x) = 2^{k/2} \sqrt{\frac{(p+k)!}{p!}}\, \psi_{p+k}(x) \quad ,$$

$$(x - \frac{d}{dx})^k (x + \frac{d}{dx})^n \psi_m(x) = 2^{(n+k)/2} \frac{\sqrt{m!(m-n+k)!}}{(m-n)!}\, \psi_{m-n+k}(x) \quad .$$

Hence from (*),

$$\Lambda\psi_m(x) = \sum_{k=0}^{\infty} \sum_{n=0}^{m} b_{kn}\, 2^{(n+k)/2} \frac{\sqrt{m!(m-n+k)!}}{(m-n)!}\, \psi_{m-n+k}(x) \quad .$$

Any term in the sum for which $n > m$ is zero, since in that case $(x + \frac{d}{dx})^n \psi_m(x) = 0$. We can recognize this by the appearance of a negative argument in the factorial. Changing the summation indices we have

$$\Lambda\psi_m(x) = \sum_{k=0}^{\infty} \sum_{\ell=k}^{m+k} b_{k,m+k-\ell}\, 2^{k+(m-\ell)/2} \frac{\sqrt{m!\ell!}}{(\ell-k)!}\, \psi_\ell(x) \quad .$$

Now let us see what coefficients in the sum contribute to $\psi_\ell(x)$ for some fixed ℓ . Since $k \le \ell \le m+k$ for a contribution, we have $\max\{0,\ell-m\} \le k \le \ell$. Thus

$$\Lambda\psi_m(x) = \sum_{\ell=0}^{\infty} \left(\sum_{k=\max\{0,\ell-m\}}^{\infty} b_{k,m+k-\ell}\, 2^{k+(m-\ell)/2}\, \frac{\sqrt{m!\,\ell!}}{(\ell-k)!} \right) \psi_\ell(x)$$

$$= \sum_{\ell=0}^{\infty} \Lambda_{\ell m}\, \psi_\ell(x) \quad ,$$

where

$$\Lambda_{\ell m} = \sum_{k=\max\{0,\ell-m\}}^{\ell} b_{k,m+k-\ell}\, 2^{k+(m-\ell)/2}\, \frac{\sqrt{m!\,\ell!}}{(\ell-k)!} \quad . \tag{1}$$

From (1) we see

$$\Lambda_{0m} = b_{0,m}\, 2^{m/2} \sqrt{m!} \quad . \tag{2}$$

Hence from (2) we can get $b_{0,m}$ for all m from Λ_{0m} . The result is $b_{0,m} = \Lambda_{0m}\, 2^{-m/2} (m!)^{-1/2}$. Taking $\ell = 1$ in (1) we get

$$\Lambda_{10} = b_{1,0}\, 2^{1/2}$$

$$\Lambda_{1m} = b_{0,m-1}\, 2^{(m-1)/2} \sqrt{m!} + b_{1,m}\, 2^{1+(m-1)/2} \sqrt{m!} \quad , \quad m \geq 1 \quad . \tag{3}$$

We can solve (3) to get

$$b_{1,0} = 2^{-1/2}\, \Lambda_{10}$$

$$b_{1m} = \frac{2^{-(1+m)/2}}{\sqrt{m!}} (\Lambda_{1m} - \sqrt{m}\, \Lambda_{0,m-1}) \quad \text{for} \quad m \geq 1 \quad .$$

We can repeat this for $\ell = 2,3$, etc., in sequence in (1). Hence it is clear that (1) can be inverted and b_{kn} can be expressed in terms of $\Lambda_{\ell m}$.

Hence every operator is of the form (*) or (†).

Usefulness of the Operator Representation

Let $\Lambda = \sum_{k=0}^{\infty} \sum_{n=0}^{\infty} a_{kn} x^k (\frac{d}{dx})^n$ be an arbitrary operator. This form for Λ is useful since it transforms analytic functions to analytic functions and general functions to general functions. Let $f(x) = \sum_{m=0}^{\infty} c_m x^m$ and $g(x) = \sum_{m=0}^{\infty} b_m \delta^{[m]}(x)$ be an analytic and general function respectively. Then $(\Lambda f)(x) = \sum_{p=0}^{\infty} (\sum_{n=0}^{\infty} \sum_{q=0}^{p} c_{q+n} a_{p-q,n} \frac{(q+n)!}{q!}) x^p$ and $(\Lambda g)(x) = \sum_{p=0}^{\infty} (\sum_{k=0}^{\infty} \sum_{n=0}^{p+k} a_{kn} (-1)^k \frac{(p+k)!}{p!} b_{p-n+k}) \delta^{[p]}(x)$ provided that the sum representing the internal coefficient converges.

Example: $\mathcal{D}^k = \sum_{n=0}^{\infty} \frac{k^n}{n!} (\frac{d}{dx})^n = e^{k \frac{d}{dx}}$ for constant k is the shift operator $(\mathcal{D}^k f)(x) = f(x+k)$ expanded in the form above for Λ. In this case $a_{0n} = \frac{k^n}{n!}$ and $a_{mn} = 0$ for $m \geq 1$. We can define T^k by $(T^k f)(x) = f(x+k)$ for any function f defined for all real numbers, differentiable or not. $\mathcal{D}^k$ and T^k agree on the domain of $\mathcal{D}^k$, but T^k is an extension of $\mathcal{D}^k$ in a very natural sense. Since the domain of $\mathcal{D}^k$ includes all polynomials, the functions, e^{ipx} for all real p, and $\psi_n(x)$ for $n = 0,1,2,3,\ldots$ which are examples of complete sets, we refer to $\mathcal{D}^k$ as the shift operator, and the expansion as holding in general, even though certain infinite linear combinations or integral superpositions of these complete sets of functions may lead to a function for which $\mathcal{D}^k$ is not properly defined or is divergent.

The Operator $\gamma(\frac{id}{dx})$.

One type of linear operator is function multiplication where $f(x)$ is transformed to $\gamma(x)\ f(x)$. Another very special type of operator is a function of $\frac{d}{dx}$ of the form $\gamma(\frac{id}{dx})$. If $\gamma(y) = \sum_{n=0}^{\infty} d_n y^n$ then $\gamma(\frac{id}{dx}) = \sum_{n=0}^{\infty} d_n (\frac{id}{dx})^n$ which is of the standard form (†) without power terms in x . $\mathcal{D}^k$ is an example of this type of operator, where $\mathcal{D}^k = e^{k\frac{d}{dk}}$. The function $\gamma(y)$ is e^{-iky} . Instead of expanding $\gamma(y)$ in powers of y , we might try expanding it in a Fourier series of functions e^{-iky} , that is

$$\gamma(y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \lambda(k)\ e^{-iky}\ dk \quad .$$

Then

$$\gamma(i\ \frac{d}{dx}) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \lambda(k)\ dk\ \mathcal{D}^k \ .$$

Hence

$$\gamma(i\ \frac{d}{dx})\ f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \lambda(k)\ dk\ f(x+k) \quad .$$

This explains how the general operator of the form $\gamma(i\ \frac{d}{dx})$ works. It transforms $f(x)$ to a linear combination of shifted forms of f through k namely $f(x+k)$, and the coefficient of $f(x+k)$ in the superposition is $\lambda(k)$ the fourier transform of γ , namely

$$\lambda(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \gamma(y)\ e^{iky}\ dy \quad .$$

Expanding e^{ikx} as a General Function.

Recall $g(x) = \sum_{n=0}^{\infty} b_n \, \delta^{[n]}(x)$ where $b_n = \frac{(-1)^n}{n!} \int_{-\infty}^{\infty} x^n g(x) \, dx$.

Taking $g(x) = e^{ikx}$ we get $b_n = \frac{(-1)^n}{n!} \int_{-\infty}^{\infty} x^n \, e^{ikx} \, dx$. Thus $b_n = \frac{i^n}{n!} 2\pi\delta^{[n]}(k)$. This gives $e^{ikx} = 2\pi \sum_{n=0}^{\infty} \frac{i^n}{n!} \delta^{[n]}(k) \, \delta^{[n]}(x)$. Thus we can expand the kernel of the Fourier transform operator as

$$\frac{e^{ikx}}{\sqrt{2\pi}} = \sqrt{2\pi} \sum_{n=0}^{\infty} \frac{i^n}{n!} \delta^{[n]}(k)\delta^{[n]}(x) \quad . \tag{4}$$

This is to be compared with

$$e^{ikx} = \sum_{n=0}^{\infty} \frac{i^n}{n!} k^n \, x^n \, ,$$

and

$$\frac{e^{ikx}}{\sqrt{2\pi}} = \sum_{n=0}^{\infty} \psi_n(k) \, i^n \, \psi_n(x) \quad .$$

It is important to remember that (4) is an operator equation and not a converging sum of numbers. In order to verify completeness of the general function expansion, it is enough to verify equation (4). This is done by showing that for functions $a(k)$ and $b(x)$ we have

$$\frac{1}{2\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{ikx} \, a(k)b(x)dxdk = \sum_{n=0}^{\infty} \frac{i^n}{n!} \int_{-\infty}^{\infty} a(k) \, \delta^{[n]}(k)dk \int_{-\infty}^{\infty} b(x) \, \delta^{[n]}(x) \, dx.$$

In turn, it is sufficient to verify this equation holds when the functions $a(k)$ and $b(x)$ are basis functions from a complete set, since the equation is linear. We choose $a(k) = e^{ipk}$ and $b(x) = e^{-iqx}$. The left hand side is

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{ikx}e^{ipk}e^{-iqx}dx\,dk = \int_{-\infty}^{\infty}\delta(k-q)e^{ipk}dk = e^{ipq} .$$

The right hand side is

$$\sum_{n=0}^{\infty}\frac{i^n}{n!}\int_{-\infty}^{\infty} e^{ipk}\,\delta^{[n]}(k)dk\int_{-\infty}^{\infty} e^{-iqx}\,\delta^{[n]}(x)dx = \sum_{n=0}^{\infty}\frac{i^n}{n!}((-i)^n p^n)(iq)^n$$

$$= \sum_{n=0}^{\infty}\frac{i^n}{n!}(pq)^n = e^{ipq} .$$

This proves (4) and hence the general function expansion is a complete expansion.

Expanding $\psi_n(x)$ as a General Function

Let $\psi_n(x) = \dfrac{1}{\sqrt{2^n n!\sqrt{\pi}}}H_n(x)\,e^{-x^2/2} = \sum_{k=0}^{\infty}\beta_k^{(n)}\,x^k$, where $\beta_k^{(n)}$ are the expansion coefficients in a power series. Recall that the Fourier transform of x^k is $i^{-k}\sqrt{2\pi}\,\delta^{[k]}(x)$, and the Fourier transform of $\psi_n(x)$ is $i^n\,\psi_n(x)$. Hence $i^n\,\psi_n(x) = \sum_{k=0}^{\infty}\beta_k^{(n)} i^{-k}\sqrt{2\pi}\,\delta^{[k]}(x)$. Thus the expansion of $\psi_n(x)$ as a general function is

$$\psi_n(x) = \sum_{k=0}^{\infty} \beta_k^{(n)} (-1)^{n+k} \sqrt{2\pi}\, \delta^{[k]}(x) .$$

But the coefficient in the expansion of a general function is always given in terms of the integral of the expanded function. Using this formula we get,

$$\beta_k^{(n)} = \frac{\psi_n^{[k]}(0)}{k!} = \frac{i^{n+k}(-1)^k}{\sqrt{2\pi}\ k!} \int_{-\infty}^{\infty} x^k \psi_n(x)\, dx .$$

Fractional Differentiation

For $\alpha \geq 0$ we seek to define $D_x^\alpha f(x)$ such that $D_x^0 f(x) = f(x)$ and $D_x^n f(x) = \frac{d^n}{dx^n} f(x)$, $n = 1,2,3,\ldots$. Suppose $f(x) = \frac{1}{\sqrt{2\pi}} g(k)\, e^{ikx}$, (integration convention). Then set $D_x^\alpha f(x) = \frac{1}{\sqrt{2\pi}} (ik)^\alpha g(k)\, e^{ikx}$. Observe that D_x^α is a linear operator. We take $(ik)^\alpha = e^{\alpha(\ln|k| + i\,\pi/2\ \operatorname{sgn} k)}$. Then D_x^α satisfies the required conditions for fractional differentiation. We have $D_x^\alpha \psi_n(x) = \phi_{n\ell}(\alpha)\, \psi_\ell(x)$ with summation for some $\phi_{n\ell}(\alpha)$. By fractionally differentiating the Fourier transform of $\psi_n(x)$ and using the properties of ψ_n we eventually get $\phi_{ns}(\alpha) = (ik)^\alpha i^{s-n}\, \psi_n(k)\, \psi_s(k)$. If $f(x) = f_n \psi_n(x)$ we get $D_x^\alpha f(x) = f_n (ik)^\alpha (-1)^n\, \psi_n(k) \frac{e^{ikx}}{\sqrt{2\pi}}$, or from this, $D_x^\alpha f(x) = f(t)(ik)^\alpha \frac{e^{ik(x-t)}}{2\pi} = f(t)\, D_x^\alpha \delta(x-t)$. Observe that summation and integration conventions apply throughout.

The Fundamental Coefficients

Assume summation and integration conventions apply. Define $a_{nk\ell} = \psi_n(x+h)\ \psi_\ell(h)\ \psi_k(x)$ and $\gamma_{nk\ell} = \psi_n(x)\ \psi_k(x)\ \psi_\ell(x)$. Then $\psi_n(x+h) = a_{nk\ell}\ \psi_\ell(h)\ \psi_k(x)$ and $\gamma_{nk\ell}\ \psi_n(x) = \psi_k(x)\ \psi_\ell(x)$ and $\gamma_{nk\ell}\ \psi_n(x)\ \psi_k(y) = \delta(x-y)\ \psi_\ell(x)$.

By Fourier transforming $\psi_n(x+h) = a_{nk\ell}\ \psi_\ell(h)\ \psi_k(x)$ with respect to x for fixed h we can show that

$$a_{nk\ell} = \sqrt{2\pi}\ i^{n-k-\ell}\ \gamma_{nk\ell}\ .$$

APPENDIX II

THE FRACTIONAL FOURIER TRANSFORM

Recall that from Appendix I some properties of the Hermite Expansion Functions are:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}} H_n(x)\, e^{-x^2/2} \quad , \quad \left(x - \frac{d}{dx}\right)\psi_n(x) = \sqrt{2(n+1)}\, \psi_{n+1}(x) \ ,$$

$$\int_{-\infty}^{\infty} \psi_n(x)\psi_m(x)\, dx = \delta_{nm} \quad , \quad \frac{e^{ikx}}{\sqrt{2\pi}} = \sum_{n=0}^{\infty} \psi_n(x)\, i^n\, \psi_n(k) \ ,$$

$$\sum_{n=0}^{\infty} \psi_n(x)\psi_n(y) = \delta(x-y) \quad , \quad i^n\psi_n(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi_n(k) e^{ikx}\, dk \ ,$$

$$\left(x + \frac{d}{dx}\right)\psi_n(x) = \sqrt{2n}\, \psi_{n-1}(x) \ .$$

The Fourier Transform operator has kernel $\frac{e^{ikx}}{\sqrt{2\pi}}$ and matrix

$$\begin{bmatrix} 1 & & & & & & & & & & & \\ & i & & & & & & & & & & \\ & & -1 & & & & & 0 & & & & \\ & & & -i & & & & & & & & \\ & & & & 1 & & & & & & & \\ & & & & & i & & & & & & \\ & & & & & & -1 & & & & & \\ & & 0 & & & & & -i & & & & \\ & & & & & & & & 1 & & & \\ & & & & & & & & & \cdot & & \\ & & & & & & & & & & \cdot & \\ & & & & & & & & & & & \cdot \end{bmatrix}$$

The Fractional Fourier Transform operator is defined by the matrix

$$\begin{bmatrix} 1 & & & & & & \\ & e^{i\alpha} & & & 0 & & \\ & & e^{2i\alpha} & & & & \\ & & & e^{3i\alpha} & & & \\ & & & & e^{4i\alpha} & & \\ & 0 & & & & \cdot & \\ & & & & & & \ddots \end{bmatrix}$$

and has the kernel $k_\alpha(x,y) = \sum_{n=0}^{\infty} \psi_n(x)\, e^{in\alpha}\, \psi_n(y)$. In this section we shall study this operator k_α and find an explicit expression for the kernel $k_\alpha(x,y)$. Observe that $k_0(x,y) = k_{2k\pi}(x,y) = \delta(x-y)$ and $k_\pi(x,y) = \delta(x+y)$, $k_{\pi/2}(x,y) = \frac{e^{ixy}}{\sqrt{2\pi}}$, $k_{3\pi/2}(x,y) = \frac{e^{-ixy}}{\sqrt{2\pi}}$. Also $\int_{-\infty}^{\infty} k_\alpha(x,y)\, k_\beta(y,z)dy = k_{\alpha+\beta}(x,z)$.

We let k_α be the operator corresponding to the kernel $k_\alpha(x,y)$. k_α is the Fractional Fourier transform operator. $k_{\pi/2}$ is the conventional Fourier transform operator, and $k_{3\pi/2}$ is its inverse.

Let us apply operators $(x + \frac{\partial}{\partial x})$ and $(x - \frac{\partial}{\partial x})$ to $k_\alpha(x,y)$. We get

$$(x + \frac{\partial}{\partial x})\, k_\alpha(x,y) = \sum_{n=0}^{\infty} \sqrt{2n}\, \psi_{n-1}(x)\, e^{in\alpha}\psi_n(y) \quad ,$$

and

$$(x - \frac{\partial}{\partial x})(x + \frac{\partial}{\partial x})k_\alpha(x,y) = \sum_{n=0}^{\infty} 2n\, \psi_n(x)\, e^{in\alpha}\, \psi_n(y)$$

$$= 2 \sum_{n=0}^{\infty} n\, \psi_n(x)\psi_n(y)\, e^{in\alpha} \quad .$$

This series is divergent, but we are to understand that the functions f to be transformed by this kernel are such that the coefficients $f_n = \int_{-\infty}^{\infty} f(x)\, \psi_n(x)\, dx$ satisfy the condition that $\sum_{n=0}^{\infty} n\, \psi_n(x)\, f_n$ is a convergent series. Similarly

$$-i \frac{\partial}{\partial\alpha} k_\alpha(x,y) = \sum_{n=0}^{\infty} n\, \psi_n(x)\, \psi_n(y)\, e^{in\alpha} .$$

Thus $-2i \frac{\partial}{\partial\alpha} k_\alpha = (x - \frac{\partial}{\partial x})(x + \frac{\partial}{\partial x})\, k_\alpha$. Also $k_\alpha(x,y) = k_\alpha(y,x)$ and $(x - \frac{\partial}{\partial x})(x + \frac{\partial}{\partial x}) k_\alpha = (x^2-1)k_\alpha - \frac{\partial^2 k_\alpha}{\partial x^2} = -2i \frac{\partial}{\partial\alpha} k_\alpha$, so

$$(x^2-1)k_\alpha - \frac{\partial^2 k_\alpha}{\partial x^2} = -2i \frac{\partial}{\partial\alpha} k_\alpha .$$

Let us consider the logarithm of the operator k_α . It is defined by $\log k_\alpha = \lim_{h \to 0} \frac{k_{\alpha h} - I}{h}$ where I is the identity. It is given by $\log k_\alpha = \sum_{n=0}^{\infty} \psi_n(x)\, in\alpha\, \psi_n(y)$, and has as a matrix the diagonal form

$$\begin{bmatrix} 0 & & & & 0 \\ & i\alpha & & & \\ & & 2i\alpha & & \\ & & & 3i\alpha & \\ & 0 & & & \ddots \end{bmatrix} .$$

Thus $-i \frac{\partial}{\partial\alpha} k_\alpha \Big|_{\alpha=0} = \frac{1}{i\alpha} \log k_\alpha$ so $\frac{\log k_\alpha}{\alpha} = \frac{\partial}{\partial\beta}(k_\beta)\Big|_{\beta=0}$. But

$\frac{\partial}{\partial\beta}(k_\beta) = \frac{i}{2}\,[(x^2-1)k_\beta - \frac{\partial^2 k_\beta}{\partial x^2}]$. Evaluating at $\beta = 0$ gives

$$\frac{\partial}{\partial\beta}(k_\beta)\Big|_{\beta=0} = \frac{i}{2}\,[(x^2-1)\delta(x-y) - \frac{\partial^2\delta}{\partial x^2}(x-y)] \quad .$$

Hence

$$\log k_\alpha = \alpha\,\frac{i}{2}\,[(x^2-1)\delta(x-y) - \frac{\partial^2\delta}{\partial x^2}(x-y)] \quad .$$

We can obtain k_α by exponentiating

$$\begin{aligned} k_\alpha = \exp(\log k_\alpha) &= \sum_{n=0}^{\infty} \frac{(\log k_\alpha)^n}{n!} \\ &= \sum_{n=0}^{\infty} \left(\frac{\alpha i}{2}\right)^n \frac{[(x^2-1)\delta(x-y) - \frac{\partial^2\delta}{\partial x^2}(x-y)]^n}{n!} \quad , \end{aligned}$$

where $[(x^2-1)\delta(x-y) - \frac{\partial^2\delta}{\partial x^2}(x-y)]^n$ indicates n-fold kernel composition. We observe that $[(x^2-1)\delta(x-y) - \frac{\partial^2\delta(x-y)}{\partial x^2}]^0 = \delta(x-y)$ and

$$[(x^2-1)\delta(x-y) - \frac{\partial^2\delta}{\partial x^2}(x-y)]^1 = (x^2-1)\delta(x-y) - \frac{\partial^2\delta}{\partial x^2}(x-y) \quad .$$

The operator $(x^2-1)\delta(x-y) - \frac{\partial^2\delta}{\partial x^2}(x-y) = \Lambda$ transforms functions as follows

$$\begin{aligned} \Lambda f(x) &= \int_{-\infty}^{\infty} [(y^2-1)\delta(y-x) - \frac{\partial^2\delta}{\partial y^2}(y-x)]\, f(y)\, dy \\ &= (x^2-1)f(x) - f''(x) = (x - \frac{d}{dx})(x + \frac{d}{dx})\, f(x) \quad . \end{aligned}$$

Therefore, $\Lambda = (x - \frac{d}{dx})(x + \frac{d}{dx})$. This gives a new expression for k_α namely

$$k_\alpha = \sum_{n=0}^{\infty} (\frac{\alpha i}{2})^n \frac{[(x - \frac{d}{dx})(x + \frac{d}{dx})]^n}{n!}$$

as an operator on functions, rather than as a kernel. Also note that the operator $\log k_\alpha$ is given by $\log k_\alpha = \frac{\alpha i}{2} (x - \frac{d}{dx})(x + \frac{d}{dx})$. Let us apply the operator $\log k_\alpha$ to the function $\frac{e^{i\beta x}}{\sqrt{2\pi}}$. If we do so we obtain $\frac{\alpha i}{2} (x^2+\beta^2-1) \frac{e^{i\beta x}}{\sqrt{2\pi}}$. Hence we see that

$$(x - \frac{d}{dx})(x + \frac{d}{dx}) \frac{e^{i\beta x}}{\sqrt{2\pi}} = (x^2+\beta^2-1) \frac{e^{i\beta x}}{\sqrt{2\pi}} .$$

Also

$$[(x - \frac{d}{dx})(x + \frac{d}{dx})]^2 \frac{e^{i\beta x}}{\sqrt{2\pi}} = (x^2+\beta^2-1)^2 \frac{e^{i\beta x}}{\sqrt{2\pi}} - 4i\beta x \frac{e^{i\beta x}}{\sqrt{2\pi}} - \frac{2e^{i\beta x}}{\sqrt{2\pi}} .$$

Evaluation of $[(x - \frac{d}{dx})(x + \frac{d}{dx})]^n \frac{e^{i\beta x}}{\sqrt{2\pi}}$ would make possible the determination of $k_\alpha (\frac{e^{i\beta x}}{\sqrt{2\pi}})$.

An alternative way of writing k_α is

$$k_\alpha = \exp (\frac{\alpha i}{2} (x - \frac{d}{dx})(x + \frac{d}{dx})) .$$

One can see that this is representable in the form

$$k_\alpha f(x) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \gamma_{nm}(\alpha)\, x^m f^{[n]}(x)$$

since $\Lambda^n f(x)$ consists of a sum of terms involving derivatives of $f(x)$ where coefficients are polynomials in x. Alternatively, as a kernel

$$k_\alpha(x,y) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \gamma_{nm}(\alpha)\, x^m \delta^{[n]}(x-y) \quad .$$

Let us determine $\gamma_{nm}(0)$.

$$\delta(x-y) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \gamma_{nm}(0)\, x^m \delta^{[n]}(x-y) \quad .$$

Thus $\gamma_{00}^{(0)} = 1$ and $\gamma_{nm}(0) = 0$ for $n \neq 0$ or $m \neq 0$.

Now

$$k_\alpha(x,y) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \gamma_{nm}(\alpha) x^m\, \delta^{[n]}(x-y) \quad .$$

Let us apply the relation $(x^2-1)k_\alpha - \frac{\partial^2 k_\alpha}{\partial x^2} = -2i \frac{\partial}{\partial \alpha} k_\alpha$ to this expression and collect coefficients of $x^m \delta^{[n]}(x-y)$. Observe that $\gamma_{nm}(\alpha) = 0$ for n or m less than 0 . We get $\gamma_{n,m-2}(\alpha) - \gamma_{n,m}(\alpha) - (m+2)(m+1)\gamma_{n,m+2}(\alpha) - 2(m+1)\gamma_{n-1,m+1}(\alpha) - \gamma_{n-2,m}(\alpha) = -2i \frac{d}{d\alpha} \gamma_{nm}(\alpha)$.

Solving these coupled differential equations of first order gives an alternative method for expressing the fractional Fourier transform kernel.

In order to obtain an explicit expression for the fractional Fourier transform kernel, we introduce the β operators. β_x operates on functions of x according to the real parameter α. It is defined by $\beta_x^\alpha\, k_\alpha(x,y) = yk_\alpha(x,y)$. Thus $k_\alpha(x,y)$ as a function of x with y as a parameter is an eigenfunction of β_x^α with eigenvalue y. β_x^α is a Hermitian operator, with a spectrum consisting of all real numbers.

Examples: $\beta_x^0 = x$ since $x\delta(x-y) = y\delta(x-y)$.

$$\beta_x^{\pi/2} = -i\frac{d}{dx} \quad \text{since} \quad -i\frac{d}{dx}\left(\frac{e^{ixy}}{\sqrt{2\pi}}\right) = y\,\frac{e^{ixy}}{\sqrt{2\pi}}\ .$$

$$\beta_x^{\pi} = -x \quad \text{since} \quad -x\delta(x+y) = y\delta(x+y)\ .$$

$$\beta_x^{3\pi/2} = i\frac{d}{dx} \quad \text{since} \quad i\frac{d}{dx}\left(\frac{e^{-ixy}}{\sqrt{2\pi}}\right) = y\,\frac{e^{ixy}}{\sqrt{2\pi}}\ .$$

From the examples above, we might speculate that $\beta_x^\alpha = (\cos\alpha)x - i(\sin\alpha)\frac{d}{dx}$. Let us check this result. We know that $k_\alpha(x,y) = \sum_{n=0}^{\infty} \psi_n(x)\, e^{in\alpha}\psi_n(y)$ and that $x\psi_n(x) = \sqrt{\frac{n}{2}}\,\psi_{n-1}(x) + \sqrt{\frac{n+1}{2}}\,\psi_{n+1}(x)$ and $\frac{d}{dx}\psi_n(x) = \sqrt{\frac{n}{2}}\,\psi_{n-1}(x) - \sqrt{\frac{n+1}{2}}\,\psi_{n+1}(x)$. We must prove $\beta_x^\alpha\, k_\alpha(x,y) = y\, k_\alpha(x,y)$. We get

$$\beta_x^\alpha k_\alpha(x,y) = [(\cos\alpha)x - i(\sin\alpha)\frac{d}{dx}] \sum_{n=0}^{\infty} \psi_n(x)\, e^{in\alpha}\psi_n(y)$$

$$= \sum_{n=0}^{\infty} \psi_n(y)e^{in\alpha}\{\cos\alpha[\sqrt{\tfrac{n}{2}}\,\psi_{n-1}(x) + \sqrt{\tfrac{n+1}{2}}\,\psi_{n+1}(x)]$$

$$- i\sin\alpha[\sqrt{\tfrac{n}{2}}\,\psi_{n-1}(x) - \sqrt{\tfrac{n+1}{2}}\,\psi_{n+1}(x)]\}$$

$$= \sum_{n=0}^{\infty} \psi_n(y)e^{i(n-1)\alpha}\sqrt{\tfrac{n}{2}}\,\psi_{n-1}(x) + \sum_{n=0}^{\infty} \psi_n(y)e^{i(n+1)\alpha}\sqrt{\tfrac{n+1}{2}}\,\psi_{n+1}(x)$$

$$= \sum_{n=0}^{\infty} \psi_{n+1}(y)e^{in\alpha}\sqrt{\frac{n+1}{2}}\,\psi_n(x) + \sum_{n=0}^{\infty} \psi_{n-1}(y)e^{in\alpha}\sqrt{\frac{n}{2}}\,\psi_n(x)$$

$$= \sum_{n=0}^{\infty} \psi_n(x)e^{in\alpha}\left[\sqrt{\frac{n}{2}}\,\psi_{n-1}(y) + \sqrt{\frac{n+1}{2}}\,\psi_{n+1}(y)\right]$$

$$= y\ k_\alpha(x,y)\ .$$

This proves that indeed the expression

$$\beta_x^\alpha = (\cos\alpha)x - i(\sin\alpha)\frac{d}{dx}$$

is correct.

Now that we have the explicit expression for β_x^α, let us search for eigenfunctions of β_x^α with real eigenvalue λ. This is the key to obtaining an explcit expression for $k_\alpha(x,y)$. From $\beta_x^\alpha f(x) = \lambda f(x)$ we get $(\cos\alpha)x\,f(x) - i(\sin\alpha)\frac{df}{dx}(x) = \lambda f(x)$. Thus

$$\frac{df}{dx} = \frac{i(\lambda - x\cos\alpha)}{\sin\alpha} f(x) \quad \text{or} \quad \frac{df}{f} = \frac{i(\lambda - x\cos\alpha)}{\sin\alpha}dx\ .$$

Integrate to get

$$\log f = \frac{i\lambda x - i\frac{x^2}{2}\cos\alpha}{\sin\alpha} + \text{constant.}$$

Thus $f(x) = A\,e^{(i\lambda x - i(x^2/2)\cos\alpha)/\sin\alpha}$. Alternatively, for $\lambda = y$,

$k_\alpha(x,y) = A(y,\alpha)\exp\left[\frac{iyx - i\frac{x^2}{2}\cos\alpha}{\sin\alpha}\right]$. Since $k_\alpha(x,y) = k_\alpha(y,x)$ we have $k_\alpha(x,y) = B(\alpha)\exp\left[\frac{ixy - i\frac{(x^2+y^2)}{2}\cos\alpha}{\sin\alpha}\right]$. It only remains to determine $B(\alpha)$. This can be found as a normalization factor since the operator k_α must preserve norm. Alternatively, $k_\alpha\psi_0 = \psi_0$ for all α, so that $k_\alpha e^{-x^2/2} = e^{-x^2/2}$, i.e., $e^{-x^2/2} = \int_{-\infty}^{\infty} k_\alpha(x,y)\, e^{-y^2/2}\,dy$. Applying this condition we determine $B(\alpha)$ from

$$e^{-x^2/2} = B(\alpha)\int_{-\infty}^{\infty}\exp\left[\frac{ixy - i\frac{(x^2+y^2)}{2}\cos\alpha}{\sin\alpha} - \frac{y^2}{2}\right]dy\ .$$

Observe that $B(\frac{\pi}{2}) = \frac{1}{\sqrt{2\pi}}$. Also $\delta(x) = \lim_{\alpha\to 0} B(\alpha)\exp\left[\frac{-ix^2}{2\alpha}\right]$, and $B(\frac{3\pi}{2}) = \frac{1}{\sqrt{2\pi}}$. We have

$$e^{-x^2/2} = B(\alpha)\int_{-\infty}^{\infty}\exp\left[\frac{ixy - i\frac{(x^2+y^2)}{2}\cos\alpha}{\sin\alpha} - \frac{y^2}{2}\right]dy\ .$$

Argument of exp in integral is

$$\frac{ix}{\sin\alpha}y - \frac{ix^2\cos\alpha}{2\sin\alpha} - \frac{i\cos\alpha}{2\sin\alpha}y^2 - \frac{y^2}{2}$$

$$= y^2\left[-\frac{1}{2} - i\frac{\cos\alpha}{2\sin\alpha}\right] + y\left[\frac{ix}{\sin\alpha}\right] - \frac{i\,x^2\cos\alpha}{2\sin\alpha}$$

$$= y^2\left[\frac{e^{-i\alpha}}{2i\sin\alpha}\right] + y\left[\frac{ix}{\sin\alpha}\right] - \frac{ix^2\cos\alpha}{2\sin\alpha}$$

$$= \frac{e^{-i\alpha}}{2i\sin\alpha}\left[y^2 - 2xe^{i\alpha}y + x^2\cos\alpha e^{i\alpha}\right]$$

$$= \frac{e^{-i\alpha}}{2i\sin\alpha}\left[(y-xe^{i\alpha})^2 - x^2e^{2i\alpha} + x^2\cos\alpha\, e^{i\alpha}\right]$$

$$= \frac{e^{-i\alpha}}{2i \sin \alpha} [(y - xe^{i\alpha})^2 - ix^2 e^{i\alpha} \sin \alpha]$$

$$= \frac{e^{-i\alpha}}{2i \sin \alpha} (y - xe^{i\alpha})^2 - \frac{x^2}{2} \quad .$$

Subsituting back into the integral we get

$$1 = B(\alpha) \int_{-\infty}^{\infty} \exp \left[\frac{e^{-i\alpha}(y-xe^{i\alpha})^2}{2 \, i \sin \alpha} \right] dy \; .$$

The x shift in the integral has no effect on the infinite limits because of the decay of $e^{-y^2/2}$ and hence we can drop the x term (or set $x=0$).

$$1 = B(\alpha) \int_{-\infty}^{\infty} \exp[-(\tfrac{i}{2} \cot \alpha + \tfrac{1}{2}) y^2] \, dy \quad .$$

Thus

$$1 = B(\alpha) \int_{-\infty}^{\infty} \exp[- \frac{\beta y^2}{2}] \, dy = B(\alpha) \sqrt{\frac{2\pi}{\beta}}$$

where $\beta = 1 + i \cot \alpha$. This means $B(\alpha) = \pm \sqrt{\frac{1 + i \cot \alpha}{2\pi}}$. We choose the branch of the square root that is consistent with $B(\frac{\pi}{2}) = B(\frac{3\pi}{2}) = \frac{1}{\sqrt{2\pi}}$. Thus $B(\alpha) = \sqrt{\frac{1 + i \cot \alpha}{2\pi}}$. This determines the kernel $k\,(x,y)$ explicitly as

$$k_\alpha(x,y) = \sqrt{\frac{1 + i \cot \alpha}{2\pi}} \exp \left[\frac{ixy - i \frac{(x^2+y^2)}{2} \cos \alpha}{\sin \alpha} \right] \; .$$

The complex square root taken in the one with positive real part.

APPENDIX III

PARTICLES UNDER THE INFLUENCE OF A POTENTIAL (HARMONIC OSCILLATOR)

We shall consider particles in one dimension under the influence of a potential, and will solve the problem completely for one special case (the harmonic oscillator).

Consider the equation

$$i\hbar \frac{\partial\psi}{\partial t}(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}(x,t) + V(x)\,\psi(x,t) \qquad (1)$$

where the potential $V(x)$ is independent of t . This is the general Schrödinger equation which determines the time dependence of the position wavefunction $\psi(x,t)$ for a particle in one dimension under the influence of a potential $V(x)$.

We attempt to obtain specific solutions by separation of variables, i.e. take $\psi(x,t) = X(x)T(t)$. Then

$$i\hbar\, X(x)\dot{T}(t) = -\frac{\hbar^2}{2m} X''(x)T(t) + V(x)X(x)T(t) .$$

Dividing by $X(x)T(t)$ gives

$$i\hbar \frac{\dot{T}(t)}{T(t)} = -\frac{\hbar^2}{2m}\frac{X''(x)}{X(x)} + V(x)$$

for all x and t . Hence the left and right hand sides are separately constant. Thus

$$i\hbar \frac{\dot{T}(t)}{T(t)} = E = -\frac{\hbar^2}{2m}\frac{X''(x)}{X(x)} + V(x) \quad .$$

Hence we get $T(t) \alpha\, e^{-iEt/\hbar}$. To obtain $X(x)$ we must solve

$$-\frac{\hbar^2}{2m} X''(x) + V(x)X(x) = EX(x) \quad . \tag{2}$$

Depending on the nature of the potential V solutions may be found for various values of E . The values of E for which solutions exist may be discrete or continuous. For the free particle we saw that a continuous spectrum of positive E values was possible. For the harmonic oscillator, on the other hand, we shall see that $V(x) = \frac{1}{2} m\omega^2 x^2$ restricts E to be of the form $E = (n + \frac{1}{2})\hbar\omega$, $n = 0,1,2,3,\ldots$.

Let $\{E_\alpha, \alpha\epsilon A\}$ denote the set of E values for which solutions to (2) exist, and let $X_{E_\alpha}(x)$ denote the corresponding solutions to (2). Then

$$X_{E_\alpha}(x)\, T_{E_\alpha}(t) = X_{E_\alpha}(x)\, e^{-i\frac{E_\alpha t}{\hbar}}$$

is a solution to (1) for each $\alpha \epsilon A$. The most general solution to (1) that can be constructed by this method is a linear combination of these solutions, so

$$\psi(x,t) = \sum_{\alpha\epsilon A} A_\alpha X_{E_\alpha}(x)\, e^{-i\frac{E_\alpha t}{\hbar}}$$

where A_α are some numerical coefficients.

Harmonic Oscillator

Take $V(x) = \frac{1}{2} m\omega^2 x^2$. Then for $\Lambda = \{0,1,2,3,4,\ldots\}$ we have $E_n = (n + \frac{1}{2})\hbar\omega$ and

$$X_n(x) = \sqrt{\beta}\, \pi_n(\beta x) \quad \text{where} \quad \beta = \sqrt{\frac{m\omega}{\hbar}}$$

and $\pi_n(x)$ are the Hermite expansion functions defined by

$$\pi_n(\gamma) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(\gamma)\, e^{-\gamma^2/2} \quad .$$

for an arbitrary dimensionless real variable γ . Hence we can solve (1) completely for the Harmonic oscillator. The solution is

$$\psi(x,t) = \sum_{n=0}^{\infty} A_n \sqrt{\beta}\, \pi_n(\beta x) e^{-i(n + \frac{1}{2})\omega t} \quad .$$

This is the position wavefunction for the harmonic oscillator. The coefficients A_n are to be determined for any specific wavefunction $\psi(x,t)$. First of all we write $X_n(x) = \sqrt{\beta}\, \pi_n(\beta x)$ and realize that these functions are orthonormal. Thus

$$\psi(x,t) = \sum_{n=0}^{\infty} A_n X_n(x)\, e^{-i(n + \frac{1}{2})\omega t} \quad .$$

Hence

$$\psi(x,t_0) = \sum_{n=0}^{\infty} [A_n\, e^{-i(n + \frac{1}{2})\omega t_0}]\, X_n(x)$$

so that $A_n e^{-i(n + \frac{1}{2})\omega t_0} = \int_{-\infty}^{\infty} \psi(\bar{x},t_0)\, X_n(\bar{x})\, d\bar{x}$. Therefore

$$A_n = e^{i(n + \frac{1}{2})\omega t_0} \int_{-\infty}^{\infty} \psi(\bar{x},t_0) X_n(\bar{x})\, d\bar{x} \; .$$

Hence

$$\psi(x,t) = \sum_{n=0}^{\infty} X_n(x)\, e^{-i(n + \frac{1}{2})\omega(t-t_0)} \int_{-\infty}^{\infty} \psi(\bar{x},t_0) X_n(\bar{x})\, d\bar{x}$$

$$= \int_{-\infty}^{\infty} \psi(\bar{x},t_0) \left(\sum_{n=0}^{\infty} X_n(x) X_n(\bar{x})\, e^{-i(n + \frac{1}{2})\omega(t-t_0)} \right) d\bar{x} \; .$$

This determines the wavefunction $\psi(x,t)$ for all t given its value at t_0 .

We have that $A_n = \int_{-\infty}^{\infty} \psi(\bar{x},0) X_n(\bar{x})\, d\bar{x}$ so A_n are the Fourier coefficients of $\psi(\bar{x},0)$ with respect to the orthonormal basis $X_n(\bar{x})$. Thus we may simply write

$$\psi(x,t) = \sum_{n=0}^{\infty} A_n X_n(x)\, e^{-i(n + \frac{1}{2})\omega t} \qquad (3)$$

and derive all properties from equation (3).

From the position wavefunction for a harmonic oscillator (equation (3)) we wish to derive some expectation values. Observe that A_n are complex numbers but that $X_n(x)$ are real valued functions. Also observe that normalization

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2\, dx = 1 \quad \text{implies} \quad \sum_{n=0}^{\infty} |A_n|^2 = 1 \; .$$

Expectation values to be considered are

$$\langle x\rangle_t \quad , \quad \langle x^2\rangle_t \quad , \quad \langle -i\hbar \frac{\partial}{\partial x}\rangle_t \quad , \quad \langle -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\rangle \quad .$$

To do this we must recall some properties of the Hermite Expansion Functions. Notice that

$$x\,X_n(x) = x\sqrt{\beta}\,\pi_n(\beta x) = \frac{(\beta x)\pi_n(\beta x)}{\sqrt{\beta}}$$

$$= \frac{1}{\sqrt{\beta}}\,[\sqrt{\frac{n}{2}}\,\pi_{n-1}(\beta x) + \sqrt{\frac{n+1}{2}}\,\pi_{n+1}\,(\beta x)]$$

$$= \frac{\sqrt{\beta}}{\beta}\,[\sqrt{\frac{n}{2}}\,\pi_{n-1}(\beta x) + \sqrt{\frac{n+1}{2}}\,\pi_{n+1}(\beta x)] \quad ,$$

so

$$x\,X_n(x) = \frac{1}{\beta}\,[\sqrt{\frac{n}{2}}\,X_{n-1}(x) + \sqrt{\frac{n+1}{2}}\,X_{n+1}(x)] \quad . \qquad (4)$$

Also

$$\frac{\partial}{\partial x}\,X_n(x) = \beta[\sqrt{\frac{n}{2}}\,X_{n-1}(x) - \sqrt{\frac{n+1}{2}}\,X_{n+1}(x)] \quad . \qquad (5)$$

Also

$$x^2X_n(x) = xxX_n(x)$$

$$= \frac{1}{\beta}\,[\sqrt{\frac{n}{2}}\,x\,X_{n-1}(x) + \sqrt{\frac{n+1}{2}}\,x\,X_{n+1}(x)]$$

$$= \frac{1}{\beta}\,[\sqrt{\frac{n}{2}}\,\frac{1}{\beta}\,(\sqrt{\frac{n-1}{2}}\,X_{n-2}(x) + \sqrt{\frac{n}{2}}\,\text{[illegible]}(x))$$

$$+\sqrt{\frac{n+1}{2}}\,(\frac{1}{\beta})(\sqrt{\frac{n+1}{2}}\,X_n(x) + \sqrt{\frac{n+2}{2}}\,X_{n+2}(x))]$$

$$= \frac{1}{\beta^2}\left[\frac{\sqrt{n(n-1)}}{2} X_{n-2}(x) + \frac{n}{2} X_n(x) + \frac{n+1}{2} X_n(x) + \frac{\sqrt{(n+1)(n+2)}}{2} X_{n+2}(x)\right] ,$$

so

$$x^2 X_n(x) = \frac{1}{\beta^2}\left[\frac{\sqrt{n(n-1)}}{2} X_{n-2}(x) + \frac{2n+1}{2} X_n(x) + \frac{\sqrt{(n+1)(n+2)}}{2} X_{n+2}(x)\right] .$$

Hence

$$x^2 X_n(x) = \frac{1}{2\beta^2}\left[\sqrt{n(n-1)}\, X_{n-2}(x) + (2n+1) X_n(x) + \sqrt{(n+1)(n+2)}\, X_{n+2}(x)\right] \quad (6)$$

$$\frac{\partial^2 X_n(x)}{\partial x^2} = \frac{\partial}{\partial x}\left\{\beta\left[\sqrt{\frac{n}{2}}\, X_{n-1}(x) - \sqrt{\frac{n+1}{2}}\, X_{n+1}(x)\right]\right\}$$

$$= \beta\sqrt{\frac{n}{2}}\, \frac{\partial}{\partial x} X_{n-1}(x) - \sqrt{\frac{n+1}{2}}\, \beta\, \frac{\partial}{\partial x} X_{n+1}(x) ,$$

so

$$\frac{\partial^2 X_n(x)}{\partial x^2} = \frac{\beta^2}{2}\left(\sqrt{n(n-1)}\, X_{n-2}(x) - (2n+1) X_n(x) + \sqrt{(n+1)(n+2)}\, X_{n+2}(x)\right) . \quad (7)$$

To get $\langle x \rangle$ we take $\langle x \rangle_t = \int_{-\infty}^{\infty} \psi^*(x,t)\, x\, \psi(x,t)\, dx$ and substitute from (3) and (4).

$$\langle x \rangle_t = \int_{-\infty}^{\infty}\left[\sum_{m=0}^{\infty} A_m^* X_m(x)\, e^{i(m + \frac{1}{2})\omega t}\right] x \left[\sum_{n=0}^{\infty} A_n X_n(x)\, e^{-i(n + \frac{1}{2})\omega t}\right] dx$$

$$= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} A_m^* A_n\, e^{i(m-n)\omega t} \int_{-\infty}^{\infty} X_m(x)\, x\, X_n(x)\, dx$$

$$= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} A_m^* A_n\, e^{i(m-n)\omega t}\, \frac{1}{\beta}\left[\sqrt{\frac{n}{2}}\, \delta_{m,n-1} + \sqrt{\frac{n+1}{2}}\, \delta_{m,n+1}\right] .$$

Hence

$$\langle x \rangle_t = \frac{2}{\beta} \sum_{n=0}^{\infty} \mathrm{Re}(A_n^* A_{n+1} e^{-i\omega t}) \sqrt{\frac{n+1}{2}} \quad . \tag{8}$$

Similarly, one obtains $\langle \frac{\partial}{\partial x} \rangle_t$ as

$$\langle \frac{\partial}{\partial x} \rangle_t = 2i\beta \sum_{n=0}^{\infty} I_m(A_n^* A_{n+1} e^{-i\omega t}) \sqrt{\frac{n+1}{2}} \quad . \tag{9}$$

For $p = -i\hbar \frac{\partial}{\partial x}$ we see that

$$\langle p \rangle_t = 2\hbar\beta \sum_{n=0}^{\infty} I_m(A_n^* A_{n+1} e^{-i\omega t}) \sqrt{\frac{n+1}{2}} \quad .$$

We now consider evaluating $\langle x^2 \rangle_t$. A similar calculation to the one above shows that

$$\langle x^2 \rangle = \frac{1}{\beta^2} \sum_{n=0}^{\infty} \mathrm{Re}(A_n^* A_{n+2} e^{-2i\omega t}) \sqrt{(n+1)(n+2)} + \frac{1}{2\beta^2} \sum_{n=0}^{\infty} (2n+1) \; |A_n|^2 \tag{10}$$

$$\langle \frac{\partial^2}{\partial x^2} \rangle = \beta^2 \sum_{n=0}^{\infty} \mathrm{Re}(A_n^* A_{n+2} e^{-2i\omega t}) \sqrt{(n+1)(n+2)} - \frac{\beta^2}{2} \sum_{n=0}^{\infty} (2n+1) \; |A_n|^2 \tag{11}$$

The expected kinetic energy is $\langle -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \rangle$ and the expected potential energy is $\langle \frac{1}{2} m \omega^2 x^2 \rangle$. Note that $\beta^2 = \frac{m\omega}{\hbar}$. Thus we see that

$$\langle -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \rangle + \langle \frac{1}{2} m \omega^2 x^2 \rangle = \frac{\hbar\omega}{2} \sum_{n=0}^{\infty} (2n+1) \; |A_n|^2 \quad .$$

Similarly, we can calculate $\langle i\hbar \frac{\partial}{\partial t} \rangle$

$$<i\hbar \frac{\partial}{\partial t}> = \int_{-\infty}^{\infty} \left(\sum_{m=0}^{\infty} A_m^* X_m(x) e^{i(m + \frac{1}{2})\omega t} \right) i\hbar \frac{\partial}{\partial t} \left(\sum_{n=0}^{\infty} A_n X_n(x) e^{-i(n + \frac{1}{2})\omega t} \right) dx$$

$$= \hbar\omega \sum_{n=0}^{\infty} A_n^* A_n \left(n + \frac{1}{2}\right) .$$

Thus we associate a probability $|A_n|^2$ with the n energy state of energy $(n + \frac{1}{2})\hbar\omega$. Observe that

$$m\omega<x> + i<p> = 2\hbar\,\beta\, e^{-i\omega t} \sum_{n=0}^{\infty} A_n^* A_{n+1} \sqrt{\frac{n+1}{2}} .$$

This gives us the nature of the time dependence of $<x>$ and $<p>$ which are real functions of t that oscillate sinusoidally with period ω . The peak amplitude of $<p>$ is

$$2\hbar\beta \left| \sum_{n=0}^{\infty} A_n^* A_{n+1} \sqrt{\frac{n+1}{2}} \right|$$

and the peak amplitude of $<x>$ is

$$\frac{2\hbar\beta}{m\omega} \left| \sum_{n=0}^{\infty} A_n^* A_{n+1} \sqrt{\frac{n+1}{2}} \right| .$$

For a classical harmonic oscillator $V = \frac{1}{2} m\omega^2 x^2$ and $F = -m\omega^2 x$ and so $-m\omega^2 x = m \frac{d^2x}{dt^2}$ meaning $\ddot{x} + \omega^2 x = 0$. The general solution is $x = A \cos(\omega t + \alpha)$ so $p = -m\omega A \sin(\omega t + \alpha)$ and $m\omega x + ip = m\omega A e^{-i\omega t} e^{-i\alpha}$. For the classical oscillator we see $m\omega x + ip$ is a complex multiple of $e^{-i\omega t}$ as is $m\omega<x> + i<p>$ in the quantum mechanical case.

The Momentum Wavefunction for the Harmonic Oscillator

The momentum wavefunction is determined as

$$\phi(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x,t)\, e^{-ikx}\, dx \quad .$$

In order to integrate this, we recall how to Fourier transform π_n and hence χ_n .

$$\phi(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Big(\sum_{n=0}^{\infty} A_n \chi_n(x) e^{-i(n + \frac{1}{2})\omega t} \Big)\, e^{-ikx}\, dx$$

$$= \sum_{n=0}^{\infty} A_n\, e^{-i(n + \frac{1}{2})\omega t}\, \frac{\sqrt{\beta}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \pi_n(\beta x) e^{-ikx}\, dx \quad .$$

Hence

$$\frac{\sqrt{\beta}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \pi_n(\beta x) e^{-ikx} dx = \frac{\sqrt{\beta}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \pi_n(u) e^{-ik\frac{u}{\beta}}\, \frac{du}{\beta} = \frac{(-i)^n}{\sqrt{\beta}}\, \pi_n(\tfrac{k}{\beta}) \quad .$$

Thus

$$\phi(k,t) = \sum_{n=0}^{\infty} A_n\, e^{-i(n + \frac{1}{2})\omega t}\, \frac{(-i)^n}{\sqrt{\beta}}\, \pi_n(\tfrac{k}{\beta}) \quad .$$

Summarizing

$$\psi(x,t) = \sum_{n=0}^{\infty} A_n \sqrt{\beta}\, \pi_n(\beta x) e^{-i(n + \frac{1}{2})\omega t}$$

$$\phi(k,t) = \sum_{n=0}^{\infty} A_n \frac{(-i)^n}{\sqrt{\beta}}\, \pi_n(\tfrac{k}{\beta}) e^{-i(n + \frac{1}{2})\omega t} \quad . \tag{12}$$

The Time Shift Operator for the Position Wavefunction with the Harmonic Oscillator Potential

We have seen that

$$\psi(x,t) = \int_{-\infty}^{\infty} \psi(\bar{x},t_0)\Big(\sum_{n=0}^{\infty} \chi_n(x)\chi_n(\bar{x})e^{-i(n+\frac{1}{2})\omega(t-t_0)}\Big)d\bar{x} \quad .$$

The kernel

$$\sum_{n=0}^{\infty} \beta\ \pi_n(\beta x)\pi_n(\beta\bar{x})\ e^{-i(n+\frac{1}{2})\omega(t-t_0)}$$

is the time shift kernel $\tau_{t-t_0}(x,\bar{x})$ for the harmonic oscillator position wavefunction. We have

$$\tau_{(t-t_0)}(x,\bar{x}) = \sum_{n=0}^{\infty} \beta\pi_n(\beta x)\pi_n(\beta\bar{x})\ e^{-i(n+\frac{1}{2})\omega(t-t_0)}$$

$$= \beta\ e^{-i\frac{\omega}{2}(t-t_0)} \sum_{n=0}^{\infty} \pi_n(\beta x)\pi_n(\beta\bar{x})\ e^{-in\omega(t-t_0)}$$

$$\tau_{(t-t_0)}(x,\bar{x}) = \beta\ e^{-i\frac{\omega}{2}(t-t_0)}\ k_{-\omega(t-t_0)}(\beta x,\beta\bar{x}) \quad . \tag{13}$$

Here, k is the fractional Fourier transform operator. We can substitute the explicit form for the Fractional Fourier transform kernel to get

$$\tau_{(t-t_0)}(x,\bar{x}) = \beta\ e^{-i\frac{\omega}{2}(t-t_0)} \sqrt{\frac{1 - i\cot(\omega(t-t_0))}{2\pi}}$$

$$\exp\left[\frac{i\beta^2 x\bar{x} - \frac{i\beta^2}{2}(x^2+\bar{x}^2)\cos(\omega(t-t_0))}{-\sin(\omega(t-t_0))}\right] \quad .$$

This proves that the harmonic oscillator wavefunction is periodic with period $\frac{2\pi}{\omega}$, that is $\psi(x,t) = \psi(x\ ,t+\frac{2\pi}{\omega})$. This can also be seen from the expansion of the time shift operator, namely

$$\tau_{(t-t_0)}(x,\bar{x}) = \sum_{n=0}^{\infty} \beta\ \pi_n(\beta x)\pi_n(\beta\bar{x})\ e^{-i(n+\frac{1}{2})\omega(t-t_0)} .$$

Time Shift Kernel for the Momentum Wavefunction

Similarly we have a time shift kernel $\sigma_{(t-t_0)}(k,\bar{k})$ for the momentum wavefunction $\phi(k,t)$. It is given by

$$\sigma_{(t-t_0)}(k,\bar{k}) = \sum_{n=0}^{\infty} \frac{1}{\beta}\ \pi_n\left(\frac{k}{\beta}\right)\ \pi_n\left(\frac{\bar{k}}{\beta}\right)\ e^{-i(n+\frac{1}{2})\omega(t-t_0)}$$

where

$$\phi(k,t) = \int_{-\infty}^{\infty} \phi(\bar{k},t_0)\sigma_{(t-t_0)}(k,\bar{k})\ d\bar{k} .$$

We obtain this by using $\phi(k,t) = \sum_{n=0}^{\infty} A_n(-i)^n\ Y_n(k)\ e^{-i(n+\frac{1}{2})\omega t}$ where $Y_n(k) = \frac{1}{\sqrt{\beta}}\ \pi_n(\frac{k}{\beta})$ are orthonormal functions. In terms of the Fractional Fourier transform,

$$\sigma_{(t-t_0)}(k,\bar{k}) = \frac{1}{\beta}\ e^{-i\frac{\omega}{2}(t-t_0)}\ k_{-\omega(t-t_0)}\left(\frac{k}{\beta}\ ,\ \frac{\bar{k}}{\beta}\right) . \tag{14}$$